Phthalic anhydride

Other names:	1,2-Benzenedicarboxylic acid anhydride
	1,2-Benzenedicarboxylic anhydride
	1,3-Dioxophthalan
	1,3-Isobenzofurandione
	1,3-Phthalandione
	Anhydrid kyseliny ftalove
	Anhydride phtalique
	Anidride ftalica
	Araldite HT 901
	ESEN
	Ftaalzuuranhydride
	Ftalanhydrid
	Ftalowy bezwodnik
	HT 901
	Isobenzofuran, 1,3-dihydro-1,3-dioxo-
	Isobenzofuran-1,3-dione
	NCI-C03601
	NSC 10431
	Phthalandione
	Phthalanhydride
	Phthalic acid anhydride
	Phthalsaeureanhydrid
	Rcra waste number U190
	Retarder AK
	Retarder ESEN
	Retarder PD
	Retarder PX
	Sconoc 7
	TGL 6525
	Vulkalent B/C
	o-Phthalic acid anhydride
Inchi:	InChI=1S/C8H4O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h1-4H
InchiKey:	LGRFSURHDFAFJT-UHFFFAOYSA-N
Formula:	C8H4O3
SMILES:	O=C1OC(=O)c2ccccc21
Mol. weight [g/mol]:	148.12
CAS:	85-44-9

Physical Properties

Property code	Value	Unit	Source
chs	-3259.40	kJ/mol	NIST Webbook
dm	5.30	debye	KDB
ea	1.28 ± 0.05	eV	NIST Webbook
ea	1.25 ± 0.09	eV	NIST Webbook
gf	-143.58	kJ/mol	Joback Method
hf	-371.80	kJ/mol	KDB
hfs	-460.37	kJ/mol	NIST Webbook
hfus	23.55	kJ/mol	Thermal analysis of phase change materials in the temperature range 120.150 .C
hsub	88.70 ± 2.30	kJ/mol	NIST Webbook
hvap	49.57	kJ/mol	Joback Method
ie	10.25 ± 0.05	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
log10ws	-1.39		Aqueous Solubility Prediction Method
logp	0.997		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=2)		KDB
pc	4760.00	kPa	KDB
rinpol	1313.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	225.33		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	225.33		NIST Webbook
rinpol	1313.00		NIST Webbook
ss	179.50	J/mol×K	NIST Webbook
ss	180.00	J/mol×K	NIST Webbook
tb	557.83 ± 0.30	K	NIST Webbook
tb	557.20	K	NIST Webbook
tb	560.00	K	KDB
tb	558.25 ± 0.30	K	NIST Webbook
tc	810.00	K	KDB
tf	404.76 ± 0.07	K	NIST Webbook
tf	404.75 ± 0.15	K	NIST Webbook
tf	404.55	K	Aqueous Solubility Prediction Method
tf	404.05 ± 0.40	K	NIST Webbook

tf	400.00 ± 1.50	K	NIST Webbook
tf	404.35 ± 0.15	K	NIST Webbook
tf	404.15 ± 0.25	K	NIST Webbook
tf	404.15	K	NIST Webbook
tf	403.73 ± 0.20	K	NIST Webbook
tf	404.00	K	KDB
tf	404.75 ± 0.07	K	NIST Webbook
tf	403.00 ± 3.00	K	NIST Webbook
vc	0.368	m3/kmol	KDB
zc	0.2600960		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.88	J/mol×K	675.71	Joback Method
cpg	257.60	J/mol×K	719.51	Joback Method
cpg	266.56	J/mol×K	763.31	Joback Method
cpg	274.75	J/mol×K	807.11	Joback Method
cpg	226.20	J/mol×K	588.10	Joback Method
cpg	237.41	J/mol×K	631.90	Joback Method
cpg	282.16	J/mol×K	850.92	Joback Method
cps	161.80	J/mol×K	298.10	NIST Webbook
cps	160.00	J/mol×K	298.15	NIST Webbook
hfust	23.09	kJ/mol	403.30	NIST Webbook
hfust	23.09	kJ/mol	403.30	NIST Webbook
hfust	22.10	kJ/mol	404.50	NIST Webbook
hsubt	88.40 ± 1.20	kJ/mol	318.00	NIST Webbook
hsubt	87.90	kJ/mol	348.00	NIST Webbook
hsubt	84.40 ± 1.20	kJ/mol	368.00	NIST Webbook
hvapt	54.10	kJ/mol	521.00	NIST Webbook
hvapt	63.90 ± 2.50	kJ/mol	430.50	NIST Webbook
hvapt	52.10	kJ/mol	482.50	NIST Webbook
hvapt	87.90	kJ/mol	298.15	The effect of ketone groups on the energetic properties of phthalan derivatives

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65238e+01
Coeff. B	-5.76785e+03
Coeff. C	-7.27290e+01
Temperature range (K), min.	427.98
Temperature range (K), max.	587.15

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solid-Liquid Equilibrium and Phase Diagram for Ternary 2-Methyl-1,4-naphthoquinone + Phthalic Anhydride +1,4-Dioxane System:	https://www.doi.org/10.1021/acs.jced.7b00609
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85449&Units=SI
The effect of ketone groups on the energetic properties of phthalan derivatives:	https://www.doi.org/10.1016/j.jct.2015.12.018
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Solid-liquid equilibrium and phase diagram for the ternary (2-naphthaldehyde +o-phthalic anhydride + 1,4-dioxane) system:	https://www.doi.org/10.1016/j.jct.2016.06.011
Thermal analysis of phase change materials in the temperature range 120–190 °C:	https://www.doi.org/10.1016/j.tca.2010.11.011
Measurement and correlation of ternary solid-liquid equilibrium of 2-methyl-1,4-naphthoquinone + phthalic anhydride + acetone system:	https://www.doi.org/10.1016/j.fluid.2015.09.019
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=992
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dm:	Dipole Moment
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility