Benzoic acid, anhydride

Other names: Benzoic anhydride
Benzoyl anhydride
Benzoyl benzoate
Inchi: InChI=1S/C14H10O3/c15-13(11-7-3-1-4-8-11)17-14(16)12-9-5-2-6-10-12/h1-10H
InchiKey: CHIHQLCVLOXUJW-UHFFFAOYSA-N
Formula: C14H10O3
SMILES: O=C(OC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 226.23
CAS: 93-97-0

Physical Properties

Property code	Value	Unit	Source
chs	-6523.00 ± 2.00	kJ/mol	NIST Webbook
chs	-6507.40 ± 6.70	kJ/mol	NIST Webbook
gf	-71.02	kJ/mol	Joback Method
hf	-319.00 ± 4.60	kJ/mol	NIST Webbook
hfs	-415.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-430.90 ± 6.70	kJ/mol	NIST Webbook
hfus	24.48	kJ/mol	Joback Method
hsub	96.20 ± 4.20	kJ/mol	NIST Webbook
hsub	96.20 ± 4.20	kJ/mol	NIST Webbook
hvap	67.21	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	2.684		Crippen Method
mcvol	169.610	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	1953.40		NIST Webbook
rinpol	1953.40		NIST Webbook
tb	633.20	K	NIST Webbook
tb	633.20 ± 3.00	K	NIST Webbook
tb	633.00	K	NIST Webbook
tc	951.73	K	Joback Method
tf	316.30 ± 1.00	K	NIST Webbook
tf	315.00 ± 2.00	K	NIST Webbook
tf	315.00	K	NIST Webbook
tf	315.00 ± 2.00	K	NIST Webbook
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.84	J/mol×K	703.24	Joback Method
cpg	443.22	J/mol×K	744.65	Joback Method
cpg	455.39	J/mol×K	786.07	Joback Method
cpg	466.40	J/mol×K	827.48	Joback Method
cpg	476.31	J/mol×K	868.90	Joback Method
cpg	485.18	J/mol×K	910.31	Joback Method
cpg	493.07	J/mol×K	951.73	Joback Method
dvisc	0.0007929	Pa×s	469.27	Joback Method
dvisc	0.0013677	Pa×s	422.47	Joback Method
dvisc	0.0005074	Pa×s	516.06	Joback Method
dvisc	0.0003497	Pa×s	562.86	Joback Method
dvisc	0.0002552	Pa×s	609.65	Joback Method
dvisc	0.0001948	Pa×s	656.44	Joback Method
dvisc	0.0001541	Pa×s	703.24	Joback Method
hfust	17.15	kJ/mol	313.20	NIST Webbook
hfust	17.15	kJ/mol	313.20	NIST Webbook
hvapt	69.10	kJ/mol	524.50	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C93970&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume