Phenylmaleic anhydride

Other names:	2,5-Furandione, 3-phenyl-
	3-phenyl-2,5-furandione
	3-phenylfuran-2,5-dione
Inchi:	InChI=1S/C10H6O3/c11-9-6-8(10(12)13-9)7-4-2-1-3-5-7/h1-6H
InchiKey:	QZYCWJVSPFQUQC-UHFFFAOYSA-N
Formula:	C10H6O3
SMILES:	O=C1C=C(c2ccccc2)C(=O)O1
Mol. weight [g/mol]:	174.15
CAS:	36122-35-7

Physical Properties

Property code	Value	Unit	Source
ea	1.74 ± 0.04	eV	NIST Webbook
gf	-120.98	kJ/mol	Joback Method
hf	-293.47	kJ/mol	Joback Method
hfus	16.39	kJ/mol	Joback Method
hvap	54.65	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.153		Crippen Method
mcvol	121.850	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	641.56	K	Joback Method
tc	913.26	K	Joback Method
tf	393.35	K	Thermodynamic properties of phase transitions of phenyl derivatives of maleic anhydride and oxazole
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.40	J/mol×K	641.56	Joback Method
cpg	313.14	J/mol×K	686.84	Joback Method

cpg	325.79	J/mol×K	732.13	Joback Method
cpg	337.32	J/mol×K	777.41	Joback Method
cpg	347.71	J/mol×K	822.69	Joback Method
cpg	356.93	J/mol×K	867.98	Joback Method
cpg	364.93	J/mol×K	913.26	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of phase transitions of phenyl derivatives of maleic anhydride and oxazole:	https://www.doi.org/10.1016/j.jct.2018.12.001
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=C36122357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume