1,2,3,6-Tetrahydrophthalimide

Other names:	1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro- «delta»4-Tetrahydrophthalimide Isoindole-1,3-dione, 3a,4,7,7a-tetrahydro- Tetrahydrophthalic acid imide Tetrahydrophthalimide 4-Cyclohexene-1,2-dicarboximide NSC 59011
Inchi:	InChI=1S/C8H9NO2/c10-7-5-3-1-2-4-6(5)8(11)9-7/h1-2,5-6H,3-4H2,(H,9,10,11)
InchiKey:	CIFFBTOJCKSRJY-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	O=C1N=C(O)C2CC=CCC12
Mol. weight [g/mol]:	151.16
CAS:	85-40-5

Physical Properties

Property code	Value	Unit	Source
gf	9.34	kJ/mol	Joback Method
hf	-196.20	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	62.13	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.066		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	625.73	K	Joback Method
tc	858.40	K	Joback Method
tf	419.86	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.91	J/mol×K	625.73	Joback Method
cpg	323.57	J/mol×K	664.51	Joback Method

cpg	336.31	J/mol×K	703.29	Joback Method
cpg	348.13	J/mol×K	742.06	Joback Method
cpg	359.03	J/mol×K	780.84	Joback Method
cpg	369.02	J/mol×K	819.62	Joback Method
cpg	378.11	J/mol×K	858.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C85405&Units=SI

Legend

cpg:	Ideal gas heat capacity
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