cis-1,2,3,6-Tetrahydrophthalic anhydride

Other names:	Tetrahydrophthalic anhydride cis-4-Cyclohexene-1,2-dicarboxylic anhydride 1,3-Isobenzofurandione, 3a,4,7,7a-tetrahydro-, cis- cis-3a,4,7,7a-Tetrahydro-1,3-isobenzofurandione 3a,4,7,7a-Tetrahydro-2-benzofuran-1,3-dione, (Z)- 1,3-Isobenzofurandione, 3a,4,7,7a-tetrahydro-, (3aR,7aS)-rel-
Inchi:	InChI=1S/C8H8O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h1-2,5-6H,3-4H2/t5-,6+
InchiKey:	KMOUUZVZFBCRAM-OLQVQODUSA-N
Formula:	C8H8O3
SMILES:	O=C1OC(=O)C2CC=CCC12
Mol. weight [g/mol]:	152.15
CAS:	935-79-5

Physical Properties

Property code	Value	Unit	Source
chs	-3519.00 ± 2.00	kJ/mol	NIST Webbook
gf	-199.66	kJ/mol	Joback Method
hf	-430.95	kJ/mol	Joback Method
hfs	-772.00 ± 2.00	kJ/mol	NIST Webbook
hfus	14.67	kJ/mol	Joback Method
hvap	47.04	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.652		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	570.48	K	Joback Method
tc	825.93	K	Joback Method
tf	369.01	K	Joback Method
tt	371.60 ± 1.50	K	NIST Webbook
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	340.45	J/mol×K	783.36	Joback Method
cpg	272.11	J/mol×K	570.48	Joback Method
cpg	287.75	J/mol×K	613.06	Joback Method
cpg	302.42	J/mol×K	655.63	Joback Method
cpg	316.11	J/mol×K	698.21	Joback Method
cpg	328.79	J/mol×K	740.78	Joback Method
cpg	351.08	J/mol×K	825.93	Joback Method
hsubt	53.10 ± 0.20	kJ/mol	325.00	NIST Webbook
hvapt	53.10 ± 0.10	kJ/mol	425.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C935795&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
hsubt:	Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume