3,4,5,6-Tetrahydrophthalic anhydride

Other names: 1,3-Isobenzofurandione, 4,5,6,7-tetrahydro-
1-Cyclohexene-1,2-dicarboxylic anhydride
Tetrahydrophthalic anhydride
Inchi: InChI=1S/C8H8O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h1-4H2
InchiKey: HMMBJOWWRLZEMI-UHFFFAOYSA-N
Formula: C8H8O3
SMILES: O=C1OC(=O)C2=C1CCCC2
Mol. weight [g/mol]: 152.15
CAS: 2426-02-0

Physical Properties

Property code	Value	Unit	Source
gf	-203.50	kJ/mol	Joback Method
hf	-413.21	kJ/mol	Joback Method
hfus	11.88	kJ/mol	Molar heat capacity and thermodynamic properties of 1-cyclohexene-1,2-dicarboxylic anhydride [C8H8O3]
hvap	48.98	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	0.940		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	589.78	K	Joback Method
tc	847.16	K	Joback Method
tf	402.53	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.56	J/mol×K	589.78	Joback Method
cpg	280.59	J/mol×K	632.68	Joback Method
cpg	293.75	J/mol×K	675.57	Joback Method

cpg	306.04	J/mol×K	718.47	Joback Method
cpg	317.44	J/mol×K	761.36	Joback Method
cpg	327.93	J/mol×K	804.26	Joback Method
cpg	337.51	J/mol×K	847.16	Joback Method
hfust	11.88	kJ/mol	220.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	442.00 ± 1.00	K	3.30	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=C2426020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Molar heat capacity and thermodynamic properties of 1-cyclohexene-1,2-dicarboxylic anhydride [C8H8O3]:	https://www.doi.org/10.1016/j.jct.2004.05.008

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
hfust:	Enthalpy of fusion at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume