1,4-Cyclohexadiene-1,2-dicarboxylic anhydride

Other names: 1,3-Isobenzofurandione, 4,7-dihydro-
Cyclohexa-1,4-diene-1,2-dicarboxylic acid, anhydride
Inchi: InChI=1S/C8H6O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h1-2H,3-4H2
InchiKey: XCGJCRKHWHYKIE-UHFFFAOYSA-N
Formula: C8H6O3
SMILES: O=C1OC(=O)C2=C1CC=CC2
Mol. weight [g/mol]: 150.13
CAS: 4773-89-1

Physical Properties

Property code	Value	Unit	Source
gf	-173.54	kJ/mol	Joback Method
hf	-355.43	kJ/mol	Joback Method
hfus	12.97	kJ/mol	Joback Method
hvap	49.27	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	0.716		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
pc	4553.06	kPa	Joback Method
tb	588.94	K	Joback Method
tc	849.01	K	Joback Method
tf	403.29	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.35	J/mol×K	588.94	Joback Method
cpg	258.98	J/mol×K	632.29	Joback Method
cpg	270.81	J/mol×K	675.63	Joback Method
cpg	281.83	J/mol×K	718.98	Joback Method
cpg	292.02	J/mol×K	762.32	Joback Method
cpg	301.38	J/mol×K	805.67	Joback Method
cpg	309.88	J/mol×K	849.01	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=C4773891&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