

cis,cis-3-Methyl-4-cyclohexene-1,2-dicarboxylic acid anhydride

InChI: InChI=1S/C9H10O3/c1-5-3-2-4-6-7(5)9(11)12-8(6)10/h2-3,5-7H,4H2,1H3/t5-,6-,7+/m1/s1
InChIKey: XPEKVUUBSDFMDR-QYNIQEEDSA-N

Formula: C9H10O3
SMILES: CC1C=CCC2C(=O)OC(=O)C12
Mol. weight [g/mol]: 166.17
CAS: 35438-82-5

Physical Properties

Property code	Value	Unit	Source
gf	-198.95	kJ/mol	Joback Method
hf	-471.93	kJ/mol	Joback Method
hfs	-199.20 ± 1.30	kJ/mol	NIST Webbook
hfus	18.33	kJ/mol	Joback Method
hvap	48.96	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.898		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	588.69	K	Joback Method
tc	838.56	K	Joback Method
tf	376.04	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.97	J/mol×K	796.92	Joback Method
cpg	321.30	J/mol×K	588.69	Joback Method
cpg	338.36	J/mol×K	630.34	Joback Method
cpg	354.38	J/mol×K	671.98	Joback Method
cpg	369.33	J/mol×K	713.63	Joback Method
cpg	383.21	J/mol×K	755.27	Joback Method
cpg	407.61	J/mol×K	838.56	Joback Method
hsubt	49.50 ± 1.00	kJ/mol	325.00	NIST Webbook

Sources

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=C35438825&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
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

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