

cis-piperitone oxide

Other names:	cis-Piperitone epoxide
Inchi:	InChI=1S/C10H16O2/c1-6(2)7-4-5-10(3)9(12-10)8(7)11/h6-7,9H,4-5H2,1-3H3/t7-,9+,10-/
InchiKey:	IAFONZHDZMCORS-FKTZTGRPSA-N
Formula:	C10H16O2
SMILES:	CC(C)C1CCC2(C)OC2C1=O
Mol. weight [g/mol]:	168.23
CAS:	4713-37-5

Physical Properties

Property code	Value	Unit	Source
gf	-81.63	kJ/mol	Joback Method
hf	-390.37	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	44.76	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.779		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1257.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1254.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1680.00		NIST Webbook
tb	535.85	K	Joback Method
tc	761.98	K	Joback Method
tf	334.27	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.36	J/mol×K	535.85	Joback Method
cpg	374.33	J/mol×K	573.54	Joback Method
cpg	391.13	J/mol×K	611.23	Joback Method
cpg	406.92	J/mol×K	648.91	Joback Method
cpg	421.82	J/mol×K	686.60	Joback Method
cpg	435.98	J/mol×K	724.29	Joback Method
cpg	449.52	J/mol×K	761.98	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=C4713375&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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