trans-piperitone oxide

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-UJNFCWOMSA-N
Formula: C10H16O2
SMILES: CC(C)C1CCC2(C)OC2C1=O
Mol. weight [g/mol]: 168.23
CAS: 57130-28-6

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	1253.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1253.00		NIST Webbook
ripol	1754.00		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:	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=C57130286&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
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