trans-Piperitenone oxide

Inchi: InChI=1S/C10H14O2/c1-6(2)7-4-5-10(3)9(12-10)8(7)11/h9H,4-5H2,1-3H3
InchiKey: AKASWINDKIEEBO-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC(C)=C1CCC2(C)OC2C1=O
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	-34.57	kJ/mol	Joback Method
hf	-298.51	kJ/mol	Joback Method
hfus	16.03	kJ/mol	Joback Method
hvap	46.33	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.843		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
tb	547.48	K	Joback Method
tc	780.47	K	Joback Method
tf	349.91	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.24	J/mol×K	547.48	Joback Method
cpg	352.30	J/mol×K	586.31	Joback Method
cpg	367.27	J/mol×K	625.14	Joback Method
cpg	381.33	J/mol×K	663.97	Joback Method
cpg	394.62	J/mol×K	702.80	Joback Method
cpg	407.32	J/mol×K	741.64	Joback Method
cpg	419.57	J/mol×K	780.47	Joback Method

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=R612758&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume