Piperitenone oxide

Inchi: InChI=1S/C10H14O2/c1-6(2)7-4-8(11)10(3)9(5-7)12-10/h7,9H,1,4-5H2,2-3H3/t7-,9-,10+/
InchiKey: YGMNGQDLUQECTO-UJNFCWOMSA-N
Formula: C10H14O2
SMILES: C=C(C)C1CC(=O)C2(C)OC2C1
Mol. weight [g/mol]: 166.22
CAS: 35178-55-3

Physical Properties

Property code	Value	Unit	Source
gf	0.10	kJ/mol	Joback Method
hf	-269.45	kJ/mol	Joback Method
hfus	15.50	kJ/mol	Joback Method
hvap	44.56	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.699		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1368.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1369.00		NIST Webbook

rinpol	1368.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1363.00		NIST Webbook
ripol	1983.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	1983.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	1984.00		NIST Webbook
tb	532.85	K	Joback Method
tc	763.26	K	Joback Method
tf	333.55	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.75	J/mol×K	532.85	Joback Method
cpg	353.90	J/mol×K	571.25	Joback Method
cpg	369.88	J/mol×K	609.65	Joback Method
cpg	384.83	J/mol×K	648.05	Joback Method
cpg	398.91	J/mol×K	686.46	Joback Method
cpg	412.27	J/mol×K	724.86	Joback Method
cpg	425.06	J/mol×K	763.26	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=C35178553&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