Ascaridole epoxide

Inchi: InChI=1S/C10H16O3/c1-6(2)10-5-4-9(3,12-13-10)7-8(10)11-7/h6-8H,4-5H2,1-3H3
InchiKey: OBKUFMIGIUQZRU-UHFFFAOYSA-N
Formula: C10H16O3
SMILES: CC(C)C12CCC(C)(OO1)C1OC12
Mol. weight [g/mol]: 184.23
CAS: 135760-25-7

Physical Properties

Property code	Value	Unit	Source
gf	-63.92	kJ/mol	Joback Method
hf	-422.47	kJ/mol	Joback Method
hfus	24.95	kJ/mol	Joback Method
hvap	48.12	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.663		Crippen Method
mcvol	136.790	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
rinpol	1215.00		NIST Webbook
tb	524.64	K	Joback Method
tc	749.36	K	Joback Method
tf	364.55	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.38	J/mol×K	524.64	Joback Method
cpg	389.65	J/mol×K	562.09	Joback Method
cpg	405.36	J/mol×K	599.55	Joback Method
cpg	419.81	J/mol×K	637.00	Joback Method
cpg	433.30	J/mol×K	674.45	Joback Method
cpg	446.12	J/mol×K	711.91	Joback Method
cpg	458.59	J/mol×K	749.36	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=C135760257&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume