cis-isoascaridole

Inchi: InChI=1S/C10H16O2/c1-8(2)10-6-4-9(3,5-7-10)11-12-10/h4,6,8H,5,7H2,1-3H3/t9-,10+/m
InchiKey: MGYMHQJELJYRQS-VHSXEESVSA-N
Formula: C10H16O2
SMILES: CC(C)C12C=CC(C)(CC1)OO2
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-25.08	kJ/mol	Joback Method
hf	-297.47	kJ/mol	Joback Method
hfus	14.79	kJ/mol	Joback Method
hvap	44.65	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.452		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1240.00		NIST Webbook
tb	503.32	K	Joback Method
tc	731.96	K	Joback Method
tf	318.00	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.22	J/mol×K	503.32	Joback Method
cpg	354.85	J/mol×K	541.43	Joback Method
cpg	370.88	J/mol×K	579.53	Joback Method
cpg	385.59	J/mol×K	617.64	Joback Method
cpg	399.25	J/mol×K	655.74	Joback Method
cpg	412.14	J/mol×K	693.85	Joback Method
cpg	424.54	J/mol×K	731.96	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=R288147&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