

trans-isoascaridole

Inchi:	InChI=1S/C10H16O2/c1-6(2)10-5-4-9(3)7(11-9)8(10)12-10/h6-8H,4-5H2,1-3H3/t??,8?,9-
InchiKey:	LEZWCCRTFNBOBU-BMNUFHGDSA-N
Formula:	C10H16O2
SMILES:	CC(C)C12CCC3(C)OC3C1O2
Mol. weight [g/mol]:	168.23

Physical Properties

Property code	Value	Unit	Source
gf	34.30	kJ/mol	Joback Method
hf	-284.31	kJ/mol	Joback Method
hfus	19.07	kJ/mol	Joback Method
hvap	43.44	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.731		Crippen Method
mcvol	130.920	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
rinqol	1295.00		NIST Webbook
tb	493.42	K	Joback Method
tc	711.67	K	Joback Method
tf	341.50	K	Joback Method
vc	0.505	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.55	J/molxK	493.42	Joback Method
cpg	358.15	J/molxK	529.80	Joback Method
cpg	374.04	J/molxK	566.17	Joback Method
cpg	388.50	J/molxK	602.55	Joback Method
cpg	401.82	J/molxK	638.92	Joback Method
cpg	414.29	J/molxK	675.30	Joback Method
cpg	426.18	J/molxK	711.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R288236&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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