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/t7-,8+,9+
InchiKey: LEZWCCRTFNBOBU-SGIHWFKDSA-N
Formula: C10H16O2
SMILES: CC(C)C12CCC3(C)OC3C1O2
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
hfus	19.07	kJ/mol	Joback Method
logp	1.731		Crippen Method
mcvol	130.920	ml/mol	McGowan Method
rinpol	1283.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1295.00		NIST Webbook
ripol	1853.00		NIST Webbook

Temperature Dependent Properties

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

Sources

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R609133&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices