trans-ascaridole

Other names: trans-ascaridol
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-KATARQTJSA-N
Formula: C10H16O2
SMILES: CC(C)C12C=CC(C)(CC1)OO2
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
hfus	14.79	kJ/mol	Joback Method
ie	8.36	eV	Cheméo Relay (1.0)
logp	2.452		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
rinpol	1299.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1305.00		NIST Webbook
tf	300.20	K	Cheméo Relay (1.0)

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:	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=R235920&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point