trans-Ascaridolglycol

Inchi: InChI=1S/C10H18O2/c1-8(2)10(12)6-4-9(3,11)5-7-10/h4,6,8,11-12H,5,7H2,1-3H3/t9-,10-
InchiKey: WHOYVNZMAORLBI-NXEZZACHSA-N
Formula: C10H18O2
SMILES: CC(C)C1(O)C=CC(C)(O)CC1
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-207.04	kJ/mol	Joback Method
hf	-437.23	kJ/mol	Joback Method
hfus	7.84	kJ/mol	Joback Method
hvap	68.93	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.475		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook
ripol	2105.00		NIST Webbook
ripol	2105.00		NIST Webbook
tb	626.64	K	Joback Method
tc	820.71	K	Joback Method
tf	360.80	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.11	J/mol×K	626.64	Joback Method
cpg	419.81	J/mol×K	658.98	Joback Method
cpg	431.96	J/mol×K	691.33	Joback Method
cpg	443.70	J/mol×K	723.67	Joback Method
cpg	455.19	J/mol×K	756.02	Joback Method
cpg	466.56	J/mol×K	788.36	Joback Method

cpg	477.96	J/mol×K	820.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232743&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume