(3E,7E,11E)-1-Isopropyl-4,8,12-trimethylcyclotetra

Inchi: InChI=1S/C20H34O/c1-16(2)20(21)14-12-18(4)10-6-8-17(3)9-7-11-19(5)13-15-20/h8,11-
InchiKey: ZVWXZFYWLABNOW-GDVLXBNMSA-N
Formula: C20H34O
SMILES: CC1=CCCC(C)=CCC(O)(C(C)C)CCC(C)=CCC1
Mol. weight [g/mol]: 290.48
CAS: 67921-02-2

Physical Properties

Property code	Value	Unit	Source
gf	-38.59	kJ/mol	Joback Method
hf	-454.43	kJ/mol	Joback Method
hfus	19.36	kJ/mol	Joback Method
hvap	79.92	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	5.957		Crippen Method
mcvol	274.770	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2161.70		NIST Webbook
rinpol	2161.70		NIST Webbook
tb	815.11	K	Joback Method
tc	1039.05	K	Joback Method
tf	403.94	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.64	J/mol×K	815.11	Joback Method
cpg	897.19	J/mol×K	852.43	Joback Method
cpg	918.41	J/mol×K	889.76	Joback Method
cpg	938.36	J/mol×K	927.08	Joback Method
cpg	957.12	J/mol×K	964.40	Joback Method
cpg	974.76	J/mol×K	1001.72	Joback Method
cpg	991.37	J/mol×K	1039.05	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=C67921022&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