4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-

Other names: FW 306
4,8,13-Duvatriene-1,3-Diol
Inchi: InChI=1S/C20H34O2/c1-15(2)18-10-9-16(3)7-6-8-17(4)13-19(21)14-20(5,22)12-11-18/h7
InchiKey: RIVKDDXPCFBMOV-KEBCYCLUSA-N
Formula: C20H34O2
SMILES: CC1=CC(O)CC(C)(O)C=CC(C(C)C)CCC(C)=CCC1
Mol. weight [g/mol]: 306.48
CAS: 7220-78-2

Physical Properties

Property code	Value	Unit	Source
gf	-181.20	kJ/mol	Joback Method
hf	-635.87	kJ/mol	Joback Method
hfus	25.98	kJ/mol	Joback Method
hvap	95.32	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.783		Crippen Method
mcvol	280.640	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
ripol	2955.00		NIST Webbook
ripol	2955.00		NIST Webbook
tb	892.97	K	Joback Method
tc	1108.91	K	Joback Method
tf	443.76	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.41	J/mol×K	892.97	Joback Method
cpg	973.95	J/mol×K	928.96	Joback Method
cpg	992.27	J/mol×K	964.95	Joback Method
cpg	1009.43	J/mol×K	1000.94	Joback Method
cpg	1025.49	J/mol×K	1036.93	Joback Method

cpg	1040.51	J/mol×K	1072.92	Joback Method
cpg	1054.55	J/mol×K	1108.91	Joback Method

Sources

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=C7220782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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