Cedrane diol

Inchi: InChI=1S/C16H28O2/c1-10-5-6-12-14(2,3)7-11-8-16(10,12)9-13(17)15(11,4)18/h10-13,1
InchiKey: UEBJJCFHNQKAIK-MJKBPUIPSA-N
Formula: C16H28O2
SMILES: CC1CCC2C(C)(C)CC3CC12CC(O)C3(C)O
Mol. weight [g/mol]: 252.39

Physical Properties

Property code	Value	Unit	Source
gf	-91.16	kJ/mol	Joback Method
hf	-513.75	kJ/mol	Joback Method
hfus	18.87	kJ/mol	Joback Method
hvap	80.13	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.971		Crippen Method
mcvol	215.460	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1913.00		NIST Webbook
tb	764.91	K	Joback Method
tc	969.36	K	Joback Method
tf	489.72	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.86	J/mol×K	764.91	Joback Method
cpg	747.58	J/mol×K	798.99	Joback Method
cpg	767.39	J/mol×K	833.06	Joback Method
cpg	787.59	J/mol×K	867.14	Joback Method
cpg	808.46	J/mol×K	901.21	Joback Method
cpg	830.27	J/mol×K	935.29	Joback Method
cpg	853.31	J/mol×K	969.36	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=R396817&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