(+/-) - [1S-(1«beta»,4«beta»,4a«beta»,6«alpha»,8a«alpha»,8a-decahydro-1,6-naphthalenediol

Inchi: InChI=1S/C15H28O2/c1-10(2)11-5-8-15(4,17)13-6-7-14(3,16)9-12(11)13/h10-13,16-17H,5-9H2,1-4H3/t11-,12+,13+,14+,15+/m1/s1

InchiKey: PNPPFTXWBZJPGW-AHDPXTMNSA-N

Formula: C15H28O2

SMILES: CC(C)C1CCC(C)(O)C2CCC(C)(O)CC12

Mol. weight [g/mol]: 240.38

Physical Properties

Property code	Value	Unit	Source
gf	-161.67	kJ/mol	Joback Method
hf	-572.25	kJ/mol	Joback Method
hfus	17.75	kJ/mol	Joback Method
hvap	79.24	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.971		Crippen Method
mcvol	212.230	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	1740.00		NIST Webbook
tb	743.55	K	Joback Method
tc	942.30	K	Joback Method
tf	422.33	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.30	J/mol×K	743.55	Joback Method
cpg	709.90	J/mol×K	776.67	Joback Method
cpg	728.06	J/mol×K	809.80	Joback Method
cpg	745.95	J/mol×K	842.92	Joback Method
cpg	763.74	J/mol×K	876.05	Joback Method
cpg	781.60	J/mol×K	909.17	Joback Method
cpg	799.70	J/mol×K	942.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496541&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume