Opposit-7(11)-en-1«beta»,4«beta»-diol

Inchi: InChI=1S/C15H26O2/c1-10(2)9-11-5-7-14(3)12(16)6-8-15(4,17)13(11)14/h9,11-13,16-17
InchiKey: FKMCEEHVCIIPLE-XQYPFIQKSA-N
Formula: C15H26O2
SMILES: CC(C)=CC1CCC2(C)C(O)CCC(C)(O)C12
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-75.46	kJ/mol	Joback Method
hf	-453.38	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	79.49	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	2.891		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	1756.00		NIST Webbook
rinpol	1756.00		NIST Webbook
ripol	2607.00		NIST Webbook
ripol	2607.00		NIST Webbook
tb	743.76	K	Joback Method
tc	943.28	K	Joback Method
tf	421.81	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.13	J/mol×K	743.76	Joback Method
cpg	680.63	J/mol×K	777.01	Joback Method
cpg	697.82	J/mol×K	810.27	Joback Method
cpg	714.88	J/mol×K	843.52	Joback Method
cpg	732.01	J/mol×K	876.77	Joback Method
cpg	749.38	J/mol×K	910.03	Joback Method

cpg	767.19	J/mol×K	943.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229717&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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