8-«alpha»,11-Elemenadiol

Inchi: InChI=1S/C15H30O2/c1-7-15(6)9-13(16)12(14(4,5)17)8-11(15)10(2)3/h10-13,16-17H,7-9
InchiKey: RTCSGAWDINSXEN-RGCMKSIDSA-N
Formula: C15H30O2
SMILES: CCC1(C)CC(O)C(C(C)(C)O)CC1C(C)C
Mol. weight [g/mol]: 242.40

Physical Properties

Property code	Value	Unit	Source
gf	-201.99	kJ/mol	Joback Method
hf	-662.88	kJ/mol	Joback Method
hfus	20.60	kJ/mol	Joback Method
hvap	79.01	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.217		Crippen Method
mcvol	223.090	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1741.00		NIST Webbook
tb	729.07	K	Joback Method
tc	916.81	K	Joback Method
tf	386.43	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.43	J/mol×K	729.07	Joback Method
cpg	727.16	J/mol×K	760.36	Joback Method
cpg	744.15	J/mol×K	791.65	Joback Method
cpg	760.48	J/mol×K	822.94	Joback Method
cpg	776.26	J/mol×K	854.23	Joback Method
cpg	791.56	J/mol×K	885.52	Joback Method
cpg	806.47	J/mol×K	916.81	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=R568844&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

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