Proisocalamendiol

Inchi: InChI=1S/C16H28O/c1-11(2)13-8-9-16(5,17)14-7-6-12(3)10-15(13,14)4/h11,13-14,17H,3
InchiKey: SRAIGEKKAALUNZ-HNSVSWJLSA-N
Formula: C16H28O
SMILES: C=C1CCC2C(C)(O)CCC(C(C)C)C2(C)C1
Mol. weight [g/mol]: 236.39

Physical Properties

Property code	Value	Unit	Source
gf	44.36	kJ/mol	Joback Method
hf	-336.08	kJ/mol	Joback Method
hfus	14.02	kJ/mol	Joback Method
hvap	65.25	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.166		Crippen Method
mcvol	216.150	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1587.00		NIST Webbook
tb	678.08	K	Joback Method
tc	886.16	K	Joback Method
tf	390.70	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.75	J/mol×K	678.08	Joback Method
cpg	669.28	J/mol×K	712.76	Joback Method
cpg	689.01	J/mol×K	747.44	Joback Method
cpg	708.13	J/mol×K	782.12	Joback Method
cpg	726.83	J/mol×K	816.80	Joback Method
cpg	745.32	J/mol×K	851.48	Joback Method
cpg	763.79	J/mol×K	886.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201982&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