Preisocalamendiol

Inchi: InChI=1S/C15H24O/c1-11(2)14-9-8-12(3)6-5-7-13(4)10-15(14)16/h6,11,14H,4-5,7-10H2,
InchiKey: QTFJNWQFKJITEE-SDQBBNPISA-N
Formula: C15H24O
SMILES: C=C1CCC=C(C)CCC(C(C)C)C(=O)C1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	-0.15	kJ/mol	Joback Method
hf	-335.68	kJ/mol	Joback Method
hfus	13.70	kJ/mol	Joback Method
hvap	55.07	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.294		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1587.00		NIST Webbook
rinpol	1587.00		NIST Webbook
tb	649.91	K	Joback Method
tc	883.60	K	Joback Method
tf	332.29	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.23	J/mol×K	649.91	Joback Method
cpg	586.87	J/mol×K	688.86	Joback Method
cpg	609.01	J/mol×K	727.81	Joback Method
cpg	629.62	J/mol×K	766.76	Joback Method
cpg	648.65	J/mol×K	805.70	Joback Method
cpg	666.08	J/mol×K	844.65	Joback Method
cpg	681.85	J/mol×K	883.60	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=R321105&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