2-epi-Prezizanoic acid

Inchi: InChI=1S/C15H22O2/c1-9-10-6-7-15(8-10)11(13(16)17)4-5-12(15)14(9,2)3/h10-12H,1,4-
InchiKey: ANQAQROTXVSMMN-OZTPJHRESA-N
Formula: C15H22O2
SMILES: C=C1C2CCC3(C2)C(C(=O)O)CCC3C1(C)C
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-5.59	kJ/mol	Joback Method
hf	-337.62	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	69.73	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.480		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1884.00		NIST Webbook
rinpol	1884.00		NIST Webbook
tb	707.71	K	Joback Method
tc	921.86	K	Joback Method
tf	469.34	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.02	J/mol×K	707.71	Joback Method
cpg	613.45	J/mol×K	743.40	Joback Method
cpg	630.39	J/mol×K	779.09	Joback Method
cpg	647.10	J/mol×K	814.78	Joback Method
cpg	663.83	J/mol×K	850.48	Joback Method
cpg	680.83	J/mol×K	886.17	Joback Method
cpg	698.35	J/mol×K	921.86	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=R516219&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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