Caryophyllen-5-ol III

Inchi: InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h5,12-14,16H,1,6-9
InchiKey: DWUYGFWOANEJRE-BZMNMHEJSA-N
Formula: C15H24O
SMILES: C=C1CCC(O)C(C)=CCC2C1CC2(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	52.10	kJ/mol	Joback Method
hf	-285.25	kJ/mol	Joback Method
hfus	19.98	kJ/mol	Joback Method
hvap	65.69	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	1642.00		NIST Webbook
ripol	2317.00		NIST Webbook
ripol	2317.00		NIST Webbook
tb	663.81	K	Joback Method
tc	872.81	K	Joback Method
tf	380.29	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.12	J/mol×K	663.81	Joback Method
cpg	595.62	J/mol×K	698.64	Joback Method
cpg	614.14	J/mol×K	733.48	Joback Method
cpg	631.79	J/mol×K	768.31	Joback Method
cpg	648.66	J/mol×K	803.14	Joback Method
cpg	664.87	J/mol×K	837.98	Joback Method
cpg	680.52	J/mol×K	872.81	Joback Method

Sources

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=R545747&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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