

Caryophyllene alcohol

Inchi: InChI=1S/C15H26O/c1-13(2)9-12-11(13)5-8-14(3)6-4-7-15(12,16)10-14/h11-12,16H,4-10H
InchiKey: FUQAYSQLAOJBBC-UHFFFAOYSA-N
Formula: C15H26O
SMILES: CC12CCCC(O)(C1)C1CC(C)(C)C1CC2
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	52.66	kJ/mol	Joback Method
hf	-300.20	kJ/mol	Joback Method
hfus	10.05	kJ/mol	Joback Method
hvap	61.85	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.754		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1575.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1557.00		NIST Webbook
tb	659.19	K	Joback Method
tc	879.30	K	Joback Method
tf	426.11	K	Joback Method
vc	0.734	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.54	J/mol×K	659.19	Joback Method

cpg	617.00	J/mol×K	695.88	Joback Method
cpg	636.71	J/mol×K	732.56	Joback Method
cpg	656.04	J/mol×K	769.25	Joback Method
cpg	675.35	J/mol×K	805.93	Joback Method
cpg	694.99	J/mol×K	842.62	Joback Method
cpg	715.33	J/mol×K	879.30	Joback Method

Sources

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=R600394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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