

«alpha»-Humulene alcohol

Inchi:	InChI=1S/C15H26O/c1-13(2)8-10-11(9-13)15(4)7-5-6-14(10,3)12(15)16/h10-12,16H,5-9H
InchiKey:	MJYUBUQHKCAJQR-YABAYLBRSA-N
Formula:	C15H26O
SMILES:	CC1(C)CC2C(C1)C1(C)CCCC2(C)C1O
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	57.05	kJ/mol	Joback Method
hf	-314.38	kJ/mol	Joback Method
hfus	13.22	kJ/mol	Joback Method
hvap	61.37	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.610		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
ripol	2000.00		NIST Webbook
tb	650.25	K	Joback Method
tc	863.66	K	Joback Method
tf	425.39	K	Joback Method
vc	0.741	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.75	J/mol×K	650.25	Joback Method
cpg	615.74	J/mol×K	685.82	Joback Method
cpg	634.97	J/mol×K	721.39	Joback Method
cpg	653.76	J/mol×K	756.96	Joback Method
cpg	672.45	J/mol×K	792.52	Joback Method
cpg	691.37	J/mol×K	828.09	Joback Method
cpg	710.84	J/mol×K	863.66	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=R399212&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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