

Dehydroeudesmol

Inchi:	InChI=1S/C15H28O/c1-11-6-5-8-15(4)9-7-12(10-13(11)15)14(2,3)16/h11-13,16H,5-10H2
InchiKey:	YJHVMPKSUPGGPZ-FLTxFBQSA-N
Formula:	C15H28O
SMILES:	CC1CCCC2(C)CCC(C(C)(C)O)CC12
Mol. weight [g/mol]:	224.38

Physical Properties

Property code	Value	Unit	Source
gf	-6.37	kJ/mol	Joback Method
hf	-418.39	kJ/mol	Joback Method
hfus	14.99	kJ/mol	Joback Method
hvap	63.11	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.000		Crippen Method
mcvol	206.360	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook
tb	653.01	K	Joback Method
tc	862.60	K	Joback Method
tf	359.27	K	Joback Method
vc	0.761	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.48	J/mol×K	653.01	Joback Method
cpg	644.09	J/mol×K	687.94	Joback Method
cpg	664.49	J/mol×K	722.87	Joback Method
cpg	683.82	J/mol×K	757.80	Joback Method
cpg	702.24	J/mol×K	792.74	Joback Method
cpg	719.89	J/mol×K	827.67	Joback Method
cpg	736.91	J/mol×K	862.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R334220&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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