

Eudesm-4(15)-en-5-«beta»-ol

Inchi:	InChI=1S/C15H26O/c1-11(2)13-7-9-14(4)8-5-6-12(3)15(14,16)10-13/h11,13,16H,3,5-10H
InchiKey:	DIFRMHMHMLVIDPB-RBSFLKMASA-N
Formula:	C15H26O
SMILES:	C=C1CCCC2(C)CCC(C(C)C)CC12O
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	43.65	kJ/mol	Joback Method
hf	-295.10	kJ/mol	Joback Method
hfus	10.36	kJ/mol	Joback Method
hvap	63.34	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1603.00		NIST Webbook
tb	659.87	K	Joback Method
tc	871.10	K	Joback Method
tf	383.67	K	Joback Method
vc	0.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.59	J/mol×K	659.87	Joback Method
cpg	611.26	J/mol×K	695.07	Joback Method
cpg	630.08	J/mol×K	730.28	Joback Method
cpg	648.26	J/mol×K	765.48	Joback Method
cpg	666.01	J/mol×K	800.69	Joback Method
cpg	683.54	J/mol×K	835.89	Joback Method
cpg	701.06	J/mol×K	871.10	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=R199067&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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