

1,6,9-Dodecatrien-3-ol, 3,7,11-trimethyl-

Inchi:	InChI=1S/C15H26O/c1-6-15(5,16)12-8-11-14(4)10-7-9-13(2)3/h6-7,9,11,13,16H,1,8,10,1
InchiKey:	VICCDBDOBQQPNJ-DTCTWCMCSA-N
Formula:	C15H26O
SMILES:	C=CC(C)(O)CCC=C(C)CC=CC(C)C
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	178.73	kJ/mol	Joback Method
hf	-169.11	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	63.30	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.252		Crippen Method
mcvol	215.180	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	1568.40		NIST Webbook
tb	635.99	K	Joback Method
tc	817.72	K	Joback Method
tf	281.17	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.89	J/mol×K	635.99	Joback Method
cpg	591.81	J/mol×K	666.28	Joback Method
cpg	606.86	J/mol×K	696.57	Joback Method
cpg	621.13	J/mol×K	726.85	Joback Method
cpg	634.66	J/mol×K	757.14	Joback Method
cpg	647.52	J/mol×K	787.43	Joback Method
cpg	659.76	J/mol×K	817.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R515523&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
hvac:	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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