6,10-Dodecadien-1-yn-3-ol, 3,7,11-trimethyl-

Other names: Deca-4,8-dienol, 1-ethynyl-1,5,9-trimethyl-
3,7,11-trimethyldodeca-6,10-dien-1-yn-3-ol
Dehydronerolidol
Inchi: InChI=1S/C15H24O/c1-6-15(5,16)12-8-11-14(4)10-7-9-13(2)3/h1,9,11,16H,7-8,10,12H2,
InchiKey: ZNVPGYAGXVEAFP-SDNWHVSQSA-N
Formula: C15H24O
SMILES: C#CC(C)(O)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 220.35
CAS: 2387-68-0

Physical Properties

Property code	Value	Unit	Source
gf	307.85	kJ/mol	Joback Method
hf	-7.15	kJ/mol	Joback Method
hfus	32.04	kJ/mol	Joback Method
hvap	64.30	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.843		Crippen Method
mcvol	210.880	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1562.00		NIST Webbook
tb	629.75	K	Joback Method
tc	817.61	K	Joback Method
tf	330.94	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.82	J/mol×K	629.75	Joback Method
cpg	568.20	J/mol×K	661.06	Joback Method
cpg	582.72	J/mol×K	692.37	Joback Method
cpg	596.45	J/mol×K	723.68	Joback Method
cpg	609.46	J/mol×K	754.99	Joback Method

cpg	621.81	J/mol×K	786.30	Joback Method
cpg	633.58	J/mol×K	817.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2387680&Units=SI
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

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