1-Hexadecyn-3-ol, 3,7,11,15-tetramethyl-

Other names: Hexadec-1-yn-3-ol, 3,7,11,15-tetramethyl-
3,7,11,15-Tetramethyl-1-hexadecyn-3-ol
1-Hexadodecyn-3-ol, 3,7,11,15-trimethyl-
3,7,11,15-tetramethylhexadec-1-yn-3-ol
Inchi: InChI=1S/C20H38O/c1-7-20(6,21)16-10-15-19(5)14-9-13-18(4)12-8-11-17(2)3/h1,17-19,
InchiKey: MULUCORRSAVKOA-UHFFFAOYSA-N
Formula: C20H38O
SMILES: C#CC(C)(O)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 294.52
CAS: 29171-23-1

Physical Properties

Property code	Value	Unit	Source
chl	-12860.00 ± 4.50	kJ/mol	NIST Webbook
chl	-12870.00 ± 14.00	kJ/mol	NIST Webbook
chl	-12869.90	kJ/mol	NIST Webbook
gf	199.29	kJ/mol	Joback Method
hf	-341.05	kJ/mol	Joback Method
hfl	-441.10 ± 1.20	kJ/mol	NIST Webbook
hfl	-431.00 ± 14.00	kJ/mol	NIST Webbook
hfl	-431.00 ± 14.00	kJ/mol	NIST Webbook
hfus	36.64	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.810		Crippen Method
mcvol	289.930	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
ripol	2319.00		NIST Webbook
ripol	2319.00		NIST Webbook
tb	734.75	K	Joback Method
tc	912.38	K	Joback Method
tf	380.37	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.17	J/mol×K	853.17	Joback Method
cpg	961.42	J/mol×K	882.77	Joback Method
cpg	876.98	J/mol×K	734.75	Joback Method
cpg	895.61	J/mol×K	764.35	Joback Method
cpg	913.32	J/mol×K	793.96	Joback Method
cpg	930.15	J/mol×K	823.56	Joback Method
cpg	975.94	J/mol×K	912.38	Joback Method
cpl	712.70	J/mol×K	293.85	NIST Webbook
hvapt	43.80 ± 1.90	kJ/mol	430.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29171231&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

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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