1-Dodecyn-3-ol, 3,7,11-trimethyl-

Other names: 3,7,11-trimethyldodecyn-3-ol
3,7,11-Trimethyl-1-dodecyn-3-ol
Inchi: InChI=1S/C15H28O/c1-6-15(5,16)12-8-11-14(4)10-7-9-13(2)3/h1,13-14,16H,7-12H2,2-5H
InchiKey: OWRXWSVBJIIORE-UHFFFAOYSA-N
Formula: C15H28O
SMILES: C#CC(C)(O)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 224.38
CAS: 1604-35-9

Physical Properties

Property code	Value	Unit	Source
chl	-9567.30 ± 4.30	kJ/mol	NIST Webbook
chl	-9564.70	kJ/mol	NIST Webbook
chl	-9564.70 ± 8.30	kJ/mol	NIST Webbook
gf	159.63	kJ/mol	Joback Method
hf	-232.57	kJ/mol	Joback Method
hfl	-339.60 ± 8.30	kJ/mol	NIST Webbook
hfl	-337.00 ± 1.00	kJ/mol	NIST Webbook
hfl	-339.60 ± 8.30	kJ/mol	NIST Webbook
hfus	27.21	kJ/mol	Joback Method
hvap	63.45	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.003		Crippen Method
mcvol	219.480	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
ripol	1927.00		NIST Webbook
tb	620.79	K	Joback Method
tc	796.89	K	Joback Method
tf	339.02	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.37	J/mol×K	620.79	Joback Method
cpg	611.88	J/mol×K	650.14	Joback Method
cpg	627.57	J/mol×K	679.49	Joback Method
cpg	642.48	J/mol×K	708.84	Joback Method
cpg	656.64	J/mol×K	738.19	Joback Method
cpg	670.11	J/mol×K	767.54	Joback Method
cpg	682.92	J/mol×K	796.89	Joback Method
hvapt	43.20 ± 1.10	kJ/mol	462.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1604359&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
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
rinpol: Non-polar retention indices
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume