3-Dodecanol, 3,7,11-trimethyl-

Other names:	Hexahydronerolidol
	Nerolidol, hexahydro-
	3,7,11-Trimethyldodecan-3-ol
	3,7,11-Trimethyl-3-dodecanol
Inchi:	InChI=1S/C15H32O/c1-6-15(5,16)12-8-11-14(4)10-7-9-13(2)3/h13-14,16H,6-12H2,1-5H3
InchiKey:	NUKWKMGANFONQP-UHFFFAOYSA-N
Formula:	C15H32O
SMILES:	CCC(C)(O)CCCC(C)CCCC(C)C
Mol. weight [g/mol]:	228.41
CAS:	7278-65-1

Physical Properties

Property code	Value	Unit	Source
gf	-63.44	kJ/mol	Joback Method
hf	-524.47	kJ/mol	Joback Method
hfus	24.23	kJ/mol	Joback Method
hvap	63.59	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.780		Crippen Method
mcvol	228.080	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	1536.00		NIST Webbook
ripol	1797.00		NIST Webbook
tb	630.67	K	Joback Method
tc	799.11	K	Joback Method
tf	292.05	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.24	J/mol×K	630.67	Joback Method
cpg	719.46	J/mol×K	771.04	Joback Method
cpg	705.09	J/mol×K	742.96	Joback Method

cpg	690.02	J/mol×K	714.89	Joback Method
cpg	674.21	J/mol×K	686.82	Joback Method
cpg	657.63	J/mol×K	658.74	Joback Method
cpg	733.15	J/mol×K	799.11	Joback Method
dvisc	0.0000381	Pa×s	630.67	Joback Method
dvisc	0.0000685	Pa×s	574.23	Joback Method
dvisc	0.0001397	Pa×s	517.80	Joback Method
dvisc	0.0003395	Pa×s	461.36	Joback Method
dvisc	0.0010568	Pa×s	404.92	Joback Method
dvisc	0.0047515	Pa×s	348.49	Joback Method
dvisc	0.0381944	Pa×s	292.05	Joback Method

Sources

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=C7278651&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume