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

Inchi: InChI=1S/C15H30O/c1-6-15(5,16)12-8-11-14(4)10-7-9-13(2)3/h6,13-14,16H,1,7-12H2,2-
InchiKey: XLIJOVLDKFATNT-UHFFFAOYSA-N
Formula: C15H30O
SMILES: C=CC(C)(O)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 226.40
CAS: 3625-46-5

Physical Properties

Property code	Value	Unit	Source
gf	24.40	kJ/mol	Joback Method
hf	-399.04	kJ/mol	Joback Method
hfus	22.95	kJ/mol	Joback Method
hvap	62.92	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.556		Crippen Method
mcvol	223.780	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinpol	1504.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1808.00		NIST Webbook
tb	627.35	K	Joback Method
tc	797.94	K	Joback Method
tf	290.29	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.86	J/mol×K	627.35	Joback Method
cpg	634.77	J/mol×K	655.78	Joback Method
cpg	650.87	J/mol×K	684.21	Joback Method
cpg	666.19	J/mol×K	712.64	Joback Method
cpg	680.78	J/mol×K	741.07	Joback Method
cpg	694.66	J/mol×K	769.50	Joback Method

cpg	707.88	J/mol×K	797.94	Joback Method
dvisc	0.0375017	Pa×s	290.29	Joback Method
dvisc	0.0047655	Pa×s	346.47	Joback Method
dvisc	0.0010769	Pa×s	402.64	Joback Method
dvisc	0.0003503	Pa×s	458.82	Joback Method
dvisc	0.0001456	Pa×s	515.00	Joback Method
dvisc	0.0000719	Pa×s	571.17	Joback Method
dvisc	0.0000403	Pa×s	627.35	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3625465&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
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