

1,7-Octadien-3-ol, 3,7-dimethyl-

Other names:	«alpha»-Linalool 3,7-dimethyl-1,7-octadien-3-ol
Inchi:	InChI=1S/C10H18O/c1-5-10(4,11)8-6-7-9(2)3/h5,11H,1-2,6-8H2,3-4H3
InchiKey:	GYJHTGZQPKPEOT-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	C=CC(C)(O)CCCC(=C)C
Mol. weight [g/mol]:	154.25
CAS:	598-07-2

Physical Properties

Property code	Value	Unit	Source
gf	66.47	kJ/mol	Joback Method
hf	-169.64	kJ/mol	Joback Method
hfus	14.46	kJ/mol	Joback Method
hvap	51.98	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.670		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1098.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1562.00		NIST Webbook
tb	510.39	K	Joback Method
tc	685.90	K	Joback Method
tf	248.22	K	Joback Method
vc	0.567	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.21	J/mol×K	510.39	Joback Method
cpg	359.42	J/mol×K	539.64	Joback Method
cpg	371.94	J/mol×K	568.89	Joback Method
cpg	383.79	J/mol×K	598.14	Joback Method
cpg	395.03	J/mol×K	627.39	Joback Method
cpg	405.67	J/mol×K	656.64	Joback Method
cpg	415.75	J/mol×K	685.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598072&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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

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