

3,7-dimethyloct-6-enyl 4-methylvalerate

Other names:	Citronellyl isohexanoate
Inchi:	InChI=1S/C16H30O2/c1-13(2)7-6-8-15(5)11-12-18-16(17)10-9-14(3)4/h7,14-15H,6,8-12H
InchiKey:	GABKAFYIQCMDH-UHFFFAOYSA-N
Formula:	C16H30O2
SMILES:	CC(C)=CCCC(C)CCOC(=O)CCC(C)C
Mol. weight [g/mol]:	254.41
CAS:	71662-18-5

Physical Properties

Property code	Value	Unit	Source
gf	-83.29	kJ/mol	Joback Method
hf	-521.50	kJ/mol	Joback Method
hfus	31.83	kJ/mol	Joback Method
hvap	59.63	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.738		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	1686.60		NIST Webbook
rinpol	1686.60		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1663.00		NIST Webbook
tb	644.93	K	Joback Method
tc	824.65	K	Joback Method
tf	293.20	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.62	J/mol×K	644.93	Joback Method
cpg	673.89	J/mol×K	674.88	Joback Method
cpg	691.30	J/mol×K	704.84	Joback Method
cpg	707.87	J/mol×K	734.79	Joback Method

cpg	723.65	J/mol×K	764.75	Joback Method
cpg	738.64	J/mol×K	794.70	Joback Method
cpg	752.88	J/mol×K	824.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71662185&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

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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