3,7-Dimethyloct-6-en-1-yl 4-methylpentanoate

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: GABKAFYIQCMTDH-UHFFFAOYSA-N
Formula: C16H30O2
SMILES: CC(C)=CCCC(C)CCOC(=O)CCC(C)C
Mol. weight [g/mol]: 254.41

Physical Properties

Property code	Value	Unit	Source
hf	-632.68	kJ/mol	Cheméo Relay (1.0)
hfus	31.83	kJ/mol	Joback Method
hvap	73.07	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.68		Cheméo Relay (1.0)
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	550.34	K	Cheméo Relay (1.0)
tc	717.68	K	Cheméo Relay (1.0)
tf	215.35	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71662185&Units=SI

Legend

cpg:	Ideal gas heat capacity
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