

Citronellyl valerate

Other names:

Citronellyl pentanoate
3,7-dimethyloct-6-enyl valerate

Inchi: InChI=1S/C15H28O2/c1-5-6-10-15(16)17-12-11-14(4)9-7-8-13(2)3/h8,14H,5-7,9-12H2,1**InchiKey:** PFOJEJPZUVQHEH-AWEZLNQCLSA-N**Formula:** C15H28O2**SMILES:** CCCCC(=O)OCCC(C)CCC=C(C)C**Mol. weight [g/mol]:** 240.38**CAS:** 7540-53-6

Physical Properties

Property code	Value	Unit	Source
gf	-89.27	kJ/mol	Joback Method
hf	-495.58	kJ/mol	Joback Method
hfus	32.76	kJ/mol	Joback Method
hvap	57.79	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.492		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	1625.80		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1625.00		NIST Webbook
ripol	1883.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1883.00		NIST Webbook
tb	622.49	K	Joback Method
tc	800.52	K	Joback Method
tf	296.93	K	Joback Method
vc	0.875	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.69	J/mol×K	622.49	Joback Method
cpg	618.22	J/mol×K	652.16	Joback Method
cpg	634.95	J/mol×K	681.83	Joback Method
cpg	650.90	J/mol×K	711.51	Joback Method
cpg	666.10	J/mol×K	741.18	Joback Method
cpg	680.57	J/mol×K	770.85	Joback Method
cpg	694.33	J/mol×K	800.52	Joback Method

Sources

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=C7540536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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