

(3S)-(-)-Citronellal

Other names:	(S)-3,7-dimethyloct-6-enal
Inchi:	InChI=1S/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h5,8,10H,4,6-7H2,1-3H3/t10-/m1/s1
InchiKey:	NEHNMFOYXAPHSD-SNVBAGLBSA-N
Formula:	C10H18O
SMILES:	CC(C)=CCCC(C)CC=O
Mol. weight [g/mol]:	154.25
CAS:	5949-05-3

Physical Properties

Property code	Value	Unit	Source
gf	3.03	kJ/mol	Joback Method
hf	-233.16	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	44.22	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.958		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1154.00		NIST Webbook
tb	480.46	K	Joback Method
tc	663.60	K	Joback Method
tf	210.42	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.12	J/mol×K	480.46	Joback Method
cpg	340.49	J/mol×K	510.98	Joback Method
cpg	354.17	J/mol×K	541.51	Joback Method
cpg	367.20	J/mol×K	572.03	Joback Method
cpg	379.60	J/mol×K	602.55	Joback Method
cpg	391.40	J/mol×K	633.07	Joback Method
cpg	402.62	J/mol×K	663.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5949053&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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