

Citronellyl isobutyrate

Other names:

3,7-dimethyloct-6-enyl isobutyrate
Citronellyl isobutanoate
Isobutyric acid, 3,7-dimethyl-6-octenyl ester
Propanoic acid, 2-methyl-, 3,7-dimethyl-6-octenyl ester

Inchi:

InChI=1S/C14H26O2/c1-11(2)7-6-8-13(5)9-10-16-14(15)12(3)4/h7,12-13H,6,8-10H2,1-5H

InchiKey:

ZGPPERKMXSGYRK-UHFFFAOYSA-N

Formula:

C14H26O2

SMILES:

CC(C)=CCCC(C)CCOC(=O)C(C)C

Mol. weight [g/mol]:

226.35

CAS:

97-89-2

Physical Properties

Property code	Value	Unit	Source
gf	-100.13	kJ/mol	Joback Method
hf	-480.22	kJ/mol	Joback Method
hfus	26.65	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.958		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	1468.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1485.30		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1739.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1724.00		NIST Webbook

tb	599.17	K	Joback Method
tc	781.65	K	Joback Method
tf	270.66	K	Joback Method
vc	0.812	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.91	J/mol×K	599.17	Joback Method
cpg	565.30	J/mol×K	629.58	Joback Method
cpg	581.89	J/mol×K	660.00	Joback Method
cpg	597.69	J/mol×K	690.41	Joback Method
cpg	612.72	J/mol×K	720.83	Joback Method
cpg	627.03	J/mol×K	751.24	Joback Method
cpg	640.62	J/mol×K	781.65	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.28805e+01
Coeff. B	-3.86144e+03
Coeff. C	-8.37640e+01
Temperature range (K), min.	390.40
Temperature range (K), max.	593.93

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97892&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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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