Butanoic acid, 2-methyl-, 3,7-dimethyl-6-octenyl ester

Other names: 3,7-dimethyloct-6-enyl 2-methylbutyrate
Citronellyl 2-methylbutanoate

Inchi: InChI=1S/C15H28O2/c1-6-14(5)15(16)17-11-10-13(4)9-7-8-12(2)3/h8,13-14H,6-7,9-11H2

InchiKey: VLUIZCDJJSDSKM-UHFFFAOYSA-N

Formula: C15H28O2

SMILES: CCC(C)C(=O)OCCC(C)CCC=C(C)C

Mol. weight [g/mol]: 240.38

CAS: 85409-36-5

Physical Properties

Property code	Value	Unit	Source
gf	-91.71	kJ/mol	Joback Method
hf	-500.86	kJ/mol	Joback Method
hfus	29.24	kJ/mol	Joback Method
hvap	57.40	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.348		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	1587.90		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1587.90		NIST Webbook
tb	622.05	K	Joback Method
tc	803.00	K	Joback Method
tf	281.93	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.07	J/mol×K	622.05	Joback Method
cpg	618.93	J/mol×K	652.21	Joback Method
cpg	635.95	J/mol×K	682.37	Joback Method

cpg	652.16	J/mol×K	712.52	Joback Method
cpg	667.59	J/mol×K	742.68	Joback Method
cpg	682.26	J/mol×K	772.84	Joback Method
cpg	696.20	J/mol×K	803.00	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=C85409365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume