Isoamyl geranate

Other names: 3-methylbutyl (E)-3,7-dimethylocta-2,6-dienoate
Inchi: InChI=1S/C15H26O2/c1-12(2)7-6-8-14(5)11-15(16)17-10-9-13(3)4/h7,11,13H,6,8-10H2,1
InchiKey: UYYJNVGFCCTXSK-SDNWHVSQSA-N
Formula: C15H26O2
SMILES: CC(C)=CCCC(C)=CC(=O)OCCC(C)C
Mol. weight [g/mol]: 238.37
CAS: 68133-73-3

Physical Properties

Property code	Value	Unit	Source
gf	-17.60	kJ/mol	Joback Method
hf	-388.15	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	57.83	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.268		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	1650.00		NIST Webbook
ripol	1707.00		NIST Webbook
tb	626.53	K	Joback Method
tc	813.52	K	Joback Method
tf	277.89	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.04	J/mol×K	626.53	Joback Method
cpg	597.38	J/mol×K	657.69	Joback Method
cpg	613.87	J/mol×K	688.86	Joback Method
cpg	629.53	J/mol×K	720.02	Joback Method
cpg	644.42	J/mol×K	751.19	Joback Method
cpg	658.56	J/mol×K	782.35	Joback Method

cpg	671.98	J/mol×K	813.52	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C68133733&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume