5-Octen-1-ol, (Z)-, 3-methylbutanoate

Other names: (Z)-5-Octen-1-yl 3-methylbutanoate
Inchi: InChI=1S/C13H24O2/c1-4-5-6-7-8-9-10-15-13(14)11-12(2)3/h5-6,12H,4,7-11H2,1-3H3/b
InchiKey: ZWSJDKUYXLNKRR-WAYWQWQTSA-N
Formula: C13H24O2
SMILES: CCC=CCCCCOC(=O)CC(C)C
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	-97.56	kJ/mol	Joback Method
hf	-444.51	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	53.26	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.712		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	1414.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1414.00		NIST Webbook
tb	576.85	K	Joback Method
tc	755.04	K	Joback Method
tf	288.35	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.13	J/mol×K	576.85	Joback Method
cpg	512.41	J/mol×K	606.55	Joback Method
cpg	527.97	J/mol×K	636.25	Joback Method
cpg	542.83	J/mol×K	665.95	Joback Method

cpg	557.00	J/mol×K	695.64	Joback Method
cpg	570.51	J/mol×K	725.34	Joback Method
cpg	583.37	J/mol×K	755.04	Joback Method
dvisc	0.0037720	Pa×s	288.35	Joback Method
dvisc	0.0014586	Pa×s	336.43	Joback Method
dvisc	0.0007154	Pa×s	384.52	Joback Method
dvisc	0.0004110	Pa×s	432.60	Joback Method
dvisc	0.0002639	Pa×s	480.68	Joback Method
dvisc	0.0001836	Pa×s	528.77	Joback Method
dvisc	0.0001357	Pa×s	576.85	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R75688&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
dvisc: Dynamic viscosity
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

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