2-Methylbutyl octanoate

Other names: Octanoic acid, 2-methylbutyl ester
Inchi: InChI=1S/C13H26O2/c1-4-6-7-8-9-10-13(14)15-11-12(3)5-2/h12H,4-11H2,1-3H3
InchiKey: XZLBJDGPIWDVIJ-UHFFFAOYSA-N
Formula: C13H26O2
SMILES: CCCCCCCC(=O)OCC(C)CC
Mol. weight [g/mol]: 214.34
CAS: 67121-39-5

Physical Properties

Property code	Value	Unit	Source
gf	-177.78	kJ/mol	Joback Method
hf	-561.73	kJ/mol	Joback Method
hfus	28.69	kJ/mol	Joback Method
hvap	53.30	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.936		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1449.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1453.30		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1453.30		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1449.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1677.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1677.00		NIST Webbook
ripol	1657.00		NIST Webbook
tb	572.69	K	Joback Method
tc	744.36	K	Joback Method
tf	293.43	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.10	J/mol×K	572.69	Joback Method
cpg	591.64	J/mol×K	715.75	Joback Method
cpg	577.64	J/mol×K	687.14	Joback Method
cpg	563.00	J/mol×K	658.53	Joback Method
cpg	547.70	J/mol×K	629.91	Joback Method
cpg	531.74	J/mol×K	601.30	Joback Method
cpg	605.00	J/mol×K	744.36	Joback Method
dvisc	0.0001594	Pa×s	572.69	Joback Method
dvisc	0.0002152	Pa×s	526.15	Joback Method
dvisc	0.0003078	Pa×s	479.60	Joback Method
dvisc	0.0004755	Pa×s	433.06	Joback Method
dvisc	0.0008156	Pa×s	386.52	Joback Method
dvisc	0.0016218	Pa×s	339.97	Joback Method
dvisc	0.0040106	Pa×s	293.43	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C67121395&Units=SI

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