2-Methylbutyl decanoate

Inchi: InChI=1S/C15H30O2/c1-4-6-7-8-9-10-11-12-15(16)17-13-14(3)5-2/h14H,4-13H2,1-3H3
InchiKey: JRJPVFOFQVUVLG-UHFFFAOYSA-N
Formula: C15H30O2
SMILES: CCCCCCCCCC(=O)OCC(C)CC
Mol. weight [g/mol]: 242.40
CAS: 68067-33-4

Physical Properties

Property code	Value	Unit	Source
gf	-160.94	kJ/mol	Joback Method
hf	-603.01	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	57.75	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.716		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1655.70		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1655.70		NIST Webbook
ripol	1854.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1854.00		NIST Webbook
ripol	1858.00		NIST Webbook
tb	618.45	K	Joback Method
tc	788.43	K	Joback Method
tf	315.97	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	621.09	J/mol×K	618.45	Joback Method
cpg	702.28	J/mol×K	760.10	Joback Method
cpg	687.48	J/mol×K	731.77	Joback Method
cpg	671.98	J/mol×K	703.44	Joback Method
cpg	655.75	J/mol×K	675.11	Joback Method
cpg	638.80	J/mol×K	646.78	Joback Method
cpg	716.38	J/mol×K	788.43	Joback Method
dvisc	0.0001278	Pa×s	618.45	Joback Method
dvisc	0.0001735	Pa×s	568.04	Joback Method
dvisc	0.0002499	Pa×s	517.62	Joback Method
dvisc	0.0003895	Pa×s	467.21	Joback Method
dvisc	0.0006759	Pa×s	416.80	Joback Method
dvisc	0.0013649	Pa×s	366.38	Joback Method
dvisc	0.0034492	Pa×s	315.97	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=C68067334&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