Isobutyl 2-methylvalerate

Other names: Pentanoic acid, 2-methyl, 2-methylpropyl ester
Isobutyl 2-methylpentanoate
Inchi: InChI=1S/C10H20O2/c1-5-6-9(4)10(11)12-7-8(2)3/h8-9H,5-7H2,1-4H3
InchiKey: VSNXGQJZBDUEOD-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CCCC(C)C(=O)OCC(C)C
Mol. weight [g/mol]: 172.26
CAS: 6297-42-3

Physical Properties

Property code	Value	Unit	Source
gf	-205.48	kJ/mol	Joback Method
hf	-505.09	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	46.23	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.622		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1064.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1064.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1417.00		NIST Webbook
tb	503.61	K	Joback Method
tc	682.96	K	Joback Method
tf	244.62	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.51	J/mol×K	503.61	Joback Method

cpg	437.08	J/mol×K	653.07	Joback Method
cpg	424.51	J/mol×K	623.18	Joback Method
cpg	411.38	J/mol×K	593.28	Joback Method
cpg	397.67	J/mol×K	563.39	Joback Method
cpg	383.39	J/mol×K	533.50	Joback Method
cpg	449.08	J/mol×K	682.96	Joback Method
dvisc	0.0001994	Pa×s	503.61	Joback Method
dvisc	0.0002734	Pa×s	460.44	Joback Method
dvisc	0.0004002	Pa×s	417.28	Joback Method
dvisc	0.0006396	Pa×s	374.12	Joback Method
dvisc	0.0011553	Pa×s	330.95	Joback Method
dvisc	0.0024917	Pa×s	287.79	Joback Method
dvisc	0.0070487	Pa×s	244.62	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=C6297423&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