4-Methylhexyl 3-methylbutanoate

Inchi:	InChI=1S/C12H24O2/c1-5-11(4)7-6-8-14-12(13)9-10(2)3/h10-11H,5-9H2,1-4H3
InchiKey:	KQLITBHOONUXEL-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCC(C)CCCOC(=O)CC(C)C
Mol. weight [g/mol]:	200.32
CAS:	1215127-80-2

Physical Properties

Property code	Value	Unit	Source
gf	-188.64	kJ/mol	Joback Method
hf	-546.37	kJ/mol	Joback Method
hfus	22.58	kJ/mol	Joback Method
hvap	50.69	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.402		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	1311.60		NIST Webbook
tb	549.37	K	Joback Method
tc	725.46	K	Joback Method
tf	267.16	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.71	J/mol×K	549.37	Joback Method
cpg	481.08	J/mol×K	578.72	Joback Method
cpg	496.78	J/mol×K	608.07	Joback Method
cpg	511.82	J/mol×K	637.42	Joback Method
cpg	526.20	J/mol×K	666.76	Joback Method
cpg	539.94	J/mol×K	696.11	Joback Method
cpg	553.06	J/mol×K	725.46	Joback Method
dvisc	0.0062070	Pa×s	267.16	Joback Method

dvisc	0.0021594	Pa×s	314.19	Joback Method
dvisc	0.0009890	Pa×s	361.23	Joback Method
dvisc	0.0005423	Pa×s	408.26	Joback Method
dvisc	0.0003366	Pa×s	455.30	Joback Method
dvisc	0.0002285	Pa×s	502.33	Joback Method
dvisc	0.0001657	Pa×s	549.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1215127802&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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