

5-Methylhexyl 3-methylbutanoate

Inchi:	InChI=1S/C12H24O2/c1-10(2)7-5-6-8-14-12(13)9-11(3)4/h10-11H,5-9H2,1-4H3
InchiKey:	WKVQCKDXXDXRFF-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CC(C)CCCCOC(=O)CC(C)C
Mol. weight [g/mol]:	200.32
CAS:	1215127-79-9

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	1303.30		NIST Webbook
tb	549.37	K	Joback Method
tc	725.46	K	Joback Method
tf	267.16	K	Joback Method
vc	0.720	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0021594	Paxs	314.19	Joback Method
dvisc	0.0009890	Paxs	361.23	Joback Method
dvisc	0.0005423	Paxs	408.26	Joback Method
dvisc	0.0003366	Paxs	455.30	Joback Method
dvisc	0.0002285	Paxs	502.33	Joback Method
dvisc	0.0001657	Paxs	549.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1215127799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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