

Formic acid, 3-(2-methoxyethyl)heptyl ester

Inchi:	InChI=1S/C11H22O3/c1-3-4-5-11(6-8-13-2)7-9-14-10-12/h10-11H,3-9H2,1-2H3
InchiKey:	KZHUKYRURXWMAZ-UHFFFAOYSA-N
Formula:	C11H22O3
SMILES:	CCCCC(CCOC)CCOC=O
Mol. weight [g/mol]:	202.29

Physical Properties

Property code	Value	Unit	Source
gf	-270.22	kJ/mol	Joback Method
hf	-625.67	kJ/mol	Joback Method
hfus	25.39	kJ/mol	Joback Method
hvap	51.23	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.392		Crippen Method
mcvol	179.160	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinsol	1378.00		NIST Webbook
tb	544.14	K	Joback Method
tc	714.09	K	Joback Method
tf	285.19	K	Joback Method
vc	0.699	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.81	J/molxK	544.14	Joback Method
cpg	511.13	J/molxK	685.77	Joback Method
cpg	498.54	J/molxK	657.44	Joback Method
cpg	485.41	J/molxK	629.12	Joback Method
cpg	471.75	J/molxK	600.79	Joback Method
cpg	457.55	J/molxK	572.47	Joback Method
cpg	523.19	J/molxK	714.09	Joback Method
dvisc	0.0001708	Paxs	544.14	Joback Method
dvisc	0.0002279	Paxs	500.98	Joback Method

dvisc	0.0003210	Paxs	457.82	Joback Method
dvisc	0.0004856	Paxs	414.66	Joback Method
dvisc	0.0008087	Paxs	371.51	Joback Method
dvisc	0.0015402	Paxs	328.35	Joback Method
dvisc	0.0035648	Paxs	285.19	Joback Method

Sources

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=U368696&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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