Hexanoic acid, 2-methoxyethyl ester

Other names: 2-Methoxyethyl caproate
Inchi: InChI=1S/C9H18O3/c1-3-4-5-6-9(10)12-8-7-11-2/h3-8H2,1-2H3
InchiKey: WHFYLHIOEPSQJH-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: CCCCCC(=O)OCCOC
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
gf	-314.02	kJ/mol	Joback Method
hf	-606.11	kJ/mol	Joback Method
hfus	23.04	kJ/mol	Joback Method
hvap	47.19	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.756		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1183.00		NIST Webbook
rinpol	1183.00		NIST Webbook
tb	504.03	K	Joback Method
tc	677.20	K	Joback Method
tf	285.58	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.03	J/mol×K	504.03	Joback Method
cpg	361.09	J/mol×K	532.89	Joback Method
cpg	373.72	J/mol×K	561.75	Joback Method
cpg	385.91	J/mol×K	590.62	Joback Method
cpg	397.66	J/mol×K	619.48	Joback Method
cpg	408.97	J/mol×K	648.34	Joback Method
cpg	419.82	J/mol×K	677.20	Joback Method

dvisc	0.0024200	Pa×s	285.58	Joback Method
dvisc	0.0012601	Pa×s	321.99	Joback Method
dvisc	0.0007491	Pa×s	358.40	Joback Method
dvisc	0.0004902	Pa×s	394.81	Joback Method
dvisc	0.0003446	Pa×s	431.21	Joback Method
dvisc	0.0002559	Pa×s	467.62	Joback Method
dvisc	0.0001984	Pa×s	504.03	Joback Method

Sources

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=U330926&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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