Acetic acid, 2-(2-methoxyethyl)hexyl ester

Inchi: InChI=1S/C11H22O3/c1-4-5-6-11(7-8-13-3)9-14-10(2)12/h11H,4-9H2,1-3H3
InchiKey: JNNNMMJMHLESIE-UHFFFAOYSA-N
Formula: C11H22O3
SMILES: CCCCC(CCOC)COC(C)=O
Mol. weight [g/mol]: 202.29

Physical Properties

Property code	Value	Unit	Source
gf	-299.62	kJ/mol	Joback Method
hf	-652.67	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	51.26	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.392		Crippen Method
mcvol	179.160	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1352.00		NIST Webbook
tb	549.35	K	Joback Method
tc	723.04	K	Joback Method
tf	293.12	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.54	J/mol×K	549.35	Joback Method
cpg	512.28	J/mol×K	694.09	Joback Method
cpg	499.46	J/mol×K	665.14	Joback Method
cpg	486.07	J/mol×K	636.19	Joback Method
cpg	472.13	J/mol×K	607.25	Joback Method
cpg	457.61	J/mol×K	578.30	Joback Method
cpg	524.54	J/mol×K	723.04	Joback Method
dvisc	0.0001559	Pa×s	549.35	Joback Method
dvisc	0.0002079	Pa×s	506.65	Joback Method

dvisc	0.0002922	Pa×s	463.94	Joback Method
dvisc	0.0004401	Pa×s	421.24	Joback Method
dvisc	0.0007270	Pa×s	378.53	Joback Method
dvisc	0.0013647	Pa×s	335.82	Joback Method
dvisc	0.0030774	Pa×s	293.12	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=U367908&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume