Propanoic acid, 2-(1-ethoxyethoxy)-, ethyl ester

Other names: ethyl 2-(1-ethoxyethoxy)propanoate
Inchi: InChI=1S/C9H18O4/c1-5-11-8(4)13-7(3)9(10)12-6-2/h7-8H,5-6H2,1-4H3
InchiKey: PDPLXOZIQCYODY-UHFFFAOYSA-N
Formula: C9H18O4
SMILES: CCOC(=O)C(C)OC(C)OCC
Mol. weight [g/mol]: 190.24
CAS: 37101-80-7

Physical Properties

Property code	Value	Unit	Source
gf	-423.90	kJ/mol	Joback Method
hf	-748.89	kJ/mol	Joback Method
hfus	17.18	kJ/mol	Joback Method
hvap	48.83	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.337		Crippen Method
mcvol	156.850	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
ripol	1442.00		NIST Webbook
ripol	1442.00		NIST Webbook
tb	525.57	K	Joback Method
tc	705.02	K	Joback Method
tf	277.81	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.75	J/mol×K	525.57	Joback Method
cpg	387.33	J/mol×K	555.48	Joback Method
cpg	400.46	J/mol×K	585.39	Joback Method
cpg	413.12	J/mol×K	615.30	Joback Method
cpg	425.31	J/mol×K	645.21	Joback Method
cpg	437.02	J/mol×K	675.12	Joback Method

cpg	448.22	J/mol×K	705.02	Joback Method
dvisc	0.0032897	Pa×s	277.81	Joback Method
dvisc	0.0013923	Pa×s	319.10	Joback Method
dvisc	0.0007176	Pa×s	360.40	Joback Method
dvisc	0.0004238	Pa×s	401.69	Joback Method
dvisc	0.0002762	Pa×s	442.98	Joback Method
dvisc	0.0001936	Pa×s	484.28	Joback Method
dvisc	0.0001435	Pa×s	525.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37101807&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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