Butanoic acid, 3-(1-ethoxyethoxy)-2-methyl-, ethyl ester

Other names: Ethyl 3-(1-ethoxyethoxy)-2-methylbutanoate
Inchi: InChI=1S/C11H22O4/c1-6-13-10(5)15-9(4)8(3)11(12)14-7-2/h8-10H,6-7H2,1-5H3
InchiKey: PFNDFRMGKYXRMM-UHFFFAOYSA-N
Formula: C11H22O4
SMILES: CCOC(=O)C(C)C(C)OC(C)OCC
Mol. weight [g/mol]: 218.29
CAS: 86845-49-0

Physical Properties

Property code	Value	Unit	Source
gf	-409.50	kJ/mol	Joback Method
hf	-795.45	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	52.89	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.973		Crippen Method
mcvol	185.030	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
ripol	2564.00		NIST Webbook
ripol	2564.00		NIST Webbook
tb	570.89	K	Joback Method
tc	750.35	K	Joback Method
tf	285.35	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.33	J/mol×K	570.89	Joback Method
cpg	485.88	J/mol×K	600.80	Joback Method
cpg	500.83	J/mol×K	630.71	Joback Method
cpg	515.18	J/mol×K	660.62	Joback Method
cpg	528.91	J/mol×K	690.53	Joback Method
cpg	542.03	J/mol×K	720.44	Joback Method

cpg	554.51	J/mol×K	750.35	Joback Method
dvisc	0.0041094	Pa×s	285.35	Joback Method
dvisc	0.0014554	Pa×s	332.94	Joback Method
dvisc	0.0006683	Pa×s	380.53	Joback Method
dvisc	0.0003648	Pa×s	428.12	Joback Method
dvisc	0.0002248	Pa×s	475.71	Joback Method
dvisc	0.0001513	Pa×s	523.30	Joback Method
dvisc	0.0001087	Pa×s	570.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86845490&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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