2-Ethylbutyric acid, 5-methoxy-3-methylpentyl ester

Inchi: InChI=1S/C13H26O3/c1-5-12(6-2)13(14)16-10-8-11(3)7-9-15-4/h11-12H,5-10H2,1-4H3
InchiKey: SQCYWFMCZHYGDV-UHFFFAOYSA-N
Formula: C13H26O3
SMILES: CCC(CC)C(=O)OCCC(C)CCOC
Mol. weight [g/mol]: 230.34

Physical Properties

Property code	Value	Unit	Source
gf	-285.22	kJ/mol	Joback Method
hf	-699.23	kJ/mol	Joback Method
hfus	26.36	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	3.029		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
rinpol	1458.00		NIST Webbook
tb	594.67	K	Joback Method
tc	768.89	K	Joback Method
tf	300.66	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.19	J/mol×K	594.67	Joback Method
cpg	560.91	J/mol×K	623.71	Joback Method
cpg	576.94	J/mol×K	652.74	Joback Method
cpg	592.30	J/mol×K	681.78	Joback Method
cpg	606.98	J/mol×K	710.81	Joback Method
cpg	620.98	J/mol×K	739.85	Joback Method
cpg	634.32	J/mol×K	768.89	Joback Method
dvisc	0.0037201	Pa×s	300.66	Joback Method
dvisc	0.0013975	Pa×s	349.66	Joback Method

dvisc	0.0006678	Pa×s	398.66	Joback Method
dvisc	0.0003751	Pa×s	447.67	Joback Method
dvisc	0.0002361	Pa×s	496.67	Joback Method
dvisc	0.0001615	Pa×s	545.67	Joback Method
dvisc	0.0001176	Pa×s	594.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370775&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume