1-Methyl-2-methoxyethyl caproate

Inchi: InChI=1S/C10H20O3/c1-4-5-6-7-10(11)13-9(2)8-12-3/h9H,4-8H2,1-3H3
InchiKey: IEEFLNNHOLXHDU-UHFFFAOYSA-N
Formula: C10H20O3
SMILES: CCCCCC(=O)OC(C)COC
Mol. weight [g/mol]: 188.26

Physical Properties

Property code	Value	Unit	Source
gf	-308.04	kJ/mol	Joback Method
hf	-632.03	kJ/mol	Joback Method
hfus	22.11	kJ/mol	Joback Method
hvap	49.03	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.145		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1210.00		NIST Webbook
rinpol	1210.00		NIST Webbook
tb	526.47	K	Joback Method
tc	701.59	K	Joback Method
tf	281.85	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.46	J/mol×K	526.47	Joback Method
cpg	408.75	J/mol×K	555.66	Joback Method
cpg	422.52	J/mol×K	584.84	Joback Method
cpg	435.78	J/mol×K	614.03	Joback Method
cpg	448.52	J/mol×K	643.22	Joback Method
cpg	460.74	J/mol×K	672.40	Joback Method
cpg	472.44	J/mol×K	701.59	Joback Method
dvisc	0.0032312	Pa×s	281.85	Joback Method

dvisc	0.0014545	Pa×s	322.62	Joback Method
dvisc	0.0007831	Pa×s	363.39	Joback Method
dvisc	0.0004778	Pa×s	404.16	Joback Method
dvisc	0.0003191	Pa×s	444.93	Joback Method
dvisc	0.0002281	Pa×s	485.70	Joback Method
dvisc	0.0001717	Pa×s	526.47	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=R540108&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