

Octanoic acid, 2-methoxyethyl ester

Other names:	2-Methoxyethyl caprylate
Inchi:	InChI=1S/C11H22O3/c1-3-4-5-6-7-8-11(12)14-10-9-13-2/h3-10H2,1-2H3
InchiKey:	RPUOMEMMGFWBRFO-UHFFFAOYSA-N
Formula:	C11H22O3
SMILES:	CCCCCCCC(=O)OCCOC
Mol. weight [g/mol]:	202.29

Physical Properties

Property code	Value	Unit	Source
gf	-297.18	kJ/mol	Joback Method
hf	-647.39	kJ/mol	Joback Method
hfus	28.22	kJ/mol	Joback Method
hvap	51.65	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.537		Crippen Method
mvol	179.160	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1375.00		NIST Webbook
rinpol	1375.00		NIST Webbook
tb	549.79	K	Joback Method
tc	720.36	K	Joback Method
tf	308.12	K	Joback Method
vc	0.694	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.25	J/mol×K	549.79	Joback Method
cpg	510.63	J/mol×K	691.93	Joback Method
cpg	498.03	J/mol×K	663.50	Joback Method
cpg	484.89	J/mol×K	635.08	Joback Method
cpg	471.21	J/mol×K	606.65	Joback Method
cpg	457.00	J/mol×K	578.22	Joback Method
cpg	522.70	J/mol×K	720.36	Joback Method

dvisc	0.0001660	Paxs	549.79	Joback Method
dvisc	0.0002161	Paxs	509.51	Joback Method
dvisc	0.0002945	Paxs	469.23	Joback Method
dvisc	0.0004253	Paxs	428.95	Joback Method
dvisc	0.0006628	Paxs	388.68	Joback Method
dvisc	0.0011445	Paxs	348.40	Joback Method
dvisc	0.0022797	Paxs	308.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U330942&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

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