

1-Methyl-2-methoxyethyl pentadecanoate

Inchi:	InChI=1S/C19H38O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19(20)22-18(2)17-21-3/h18H
InchiKey:	AMIOMSZZYDMXOK-UHFFFAOYSA-N
Formula:	C19H38O3
SMILES:	CCCCCCCCCCCCCCC(=O)OC(C)COC
Mol. weight [g/mol]:	314.50

Physical Properties

Property code	Value	Unit	Source
gf	-232.26	kJ/mol	Joback Method
hf	-817.79	kJ/mol	Joback Method
hfus	45.42	kJ/mol	Joback Method
hvap	69.07	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.656		Crippen Method
mvol	291.880	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
rmpol	2094.00		NIST Webbook
rmpol	2094.00		NIST Webbook
tb	732.39	K	Joback Method
tc	905.15	K	Joback Method
tf	383.28	K	Joback Method
vc	1.135	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.69	J/molxK	732.39	Joback Method
cpg	900.90	J/molxK	761.18	Joback Method
cpg	919.19	J/molxK	789.98	Joback Method
cpg	936.57	J/molxK	818.77	Joback Method
cpg	953.07	J/molxK	847.57	Joback Method
cpg	968.69	J/molxK	876.36	Joback Method
cpg	983.44	J/molxK	905.15	Joback Method
dvisc	0.0015442	Paxs	383.28	Joback Method

dvisc	0.0006256	Paxs	441.46	Joback Method
dvisc	0.0003128	Paxs	499.65	Joback Method
dvisc	0.0001807	Paxs	557.84	Joback Method
dvisc	0.0001158	Paxs	616.02	Joback Method
dvisc	0.0000802	Paxs	674.20	Joback Method
dvisc	0.0000588	Paxs	732.39	Joback Method

Sources

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=R540202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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