

12,12-Dimethoxydodecanoic acid, methyl ester

Inchi:	InChI=1S/C15H30O4/c1-17-14(16)12-10-8-6-4-5-7-9-11-13-15(18-2)19-3/h15H,4-13H2,1
InchiKey:	UYESUODLZUUMGU-UHFFFAOYSA-N
Formula:	C15H30O4
SMILES:	COC(=O)CCCCCCCCCCC(OC)OC
Mol. weight [g/mol]:	274.40
CAS:	1931-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-370.94	kJ/mol	Joback Method
hf	-867.45	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	62.57	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.679		Crippen Method
mcvol	241.390	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tb	663.29	K	Joback Method
tc	833.94	K	Joback Method
tf	360.43	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.61	J/molxK	663.29	Joback Method
cpg	698.87	J/molxK	691.73	Joback Method
cpg	715.39	J/molxK	720.17	Joback Method
cpg	731.17	J/molxK	748.61	Joback Method
cpg	746.20	J/molxK	777.05	Joback Method
cpg	760.49	J/molxK	805.49	Joback Method
cpg	774.04	J/molxK	833.94	Joback Method

dvisc	0.0015473	Paxs	360.43	Joback Method
dvisc	0.0006891	Paxs	410.91	Joback Method
dvisc	0.0003664	Paxs	461.38	Joback Method
dvisc	0.0002206	Paxs	511.86	Joback Method
dvisc	0.0001455	Paxs	562.34	Joback Method
dvisc	0.0001028	Paxs	612.81	Joback Method
dvisc	0.0000765	Paxs	663.29	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=C1931675&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
mvol:	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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