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

Physical Properties

Property code	Value	Unit	Source
af	0.8142		Cheméo Relay (1.0)
hf	-912.62	kJ/mol	Cheméo Relay (1.0)
hfus	36.25	kJ/mol	Joback Method
hvap	88.00	kJ/mol	Cheméo Relay (1.0)
ie	9.40	eV	Cheméo Relay (1.0)
log10ws	-3.62		Cheméo Relay (1.0)
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	575.26	K	Cheméo Relay (1.0)
tc	747.07	K	Cheméo Relay (1.0)
tf	274.43	K	Cheméo Relay (1.0)
vc	0.921	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0015473	Pa×s	360.43	Joback Method
dvisc	0.0006891	Pa×s	410.91	Joback Method
dvisc	0.0003664	Pa×s	461.38	Joback Method
dvisc	0.0002206	Pa×s	511.86	Joback Method
dvisc	0.0001455	Pa×s	562.34	Joback Method
dvisc	0.0001028	Pa×s	612.81	Joback Method
dvisc	0.0000765	Pa×s	663.29	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1931675&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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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