

6-Octadecenoic acid, methyl ester

Other names:	Methyl 6-octadecenoate
Inchi:	InChI=1S/C19H36O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h13-14H
InchiKey:	QRTVDKVXAFJVRU-BUHFOSPRSA-N
Formula:	C19H36O2
SMILES:	CCCCCCCCCCCC=CCCCC(=O)OC
Mol. weight [g/mol]:	296.49
CAS:	52355-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-44.60	kJ/mol	Joback Method
hf	-563.07	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	67.00	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.197		Crippen Method
mcvol	281.710	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2081.00		NIST Webbook
ripol	2383.00		NIST Webbook
tb	714.57	K	Joback Method
tc	887.77	K	Joback Method
tf	370.97	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.19	J/molxK	714.57	Joback Method
cpg	844.92	J/molxK	743.44	Joback Method
cpg	862.78	J/molxK	772.30	Joback Method
cpg	879.80	J/molxK	801.17	Joback Method
cpg	896.00	J/molxK	830.04	Joback Method
cpg	911.43	J/molxK	858.90	Joback Method

cpg	926.09	J/molxK	887.77	Joback Method
dvisc	0.0017193	Paxs	370.97	Joback Method
dvisc	0.0007124	Paxs	428.24	Joback Method
dvisc	0.0003634	Paxs	485.50	Joback Method
dvisc	0.0002137	Paxs	542.77	Joback Method
dvisc	0.0001390	Paxs	600.04	Joback Method
dvisc	0.0000975	Paxs	657.30	Joback Method
dvisc	0.0000724	Paxs	714.57	Joback Method

Sources

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=C52355314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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