Heptadecanoic acid, 16-methyl-, methyl ester

Other names: Methyl isostearate
Methyl 16-methylheptadecanoate
Inchi: InChI=1S/C19H38O2/c1-18(2)16-14-12-10-8-6-4-5-7-9-11-13-15-17-19(20)21-3/h18H,4-1
InchiKey: KDQIFKKWPMBNOH-UHFFFAOYSA-N
Formula: C19H38O2
SMILES: COC(=O)CCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 298.50
CAS: 5129-61-3

Physical Properties

Property code	Value	Unit	Source
gf	-127.26	kJ/mol	Joback Method
hf	-685.57	kJ/mol	Joback Method
hfus	44.23	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	6.277		Crippen Method
mcvol	286.010	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook
rinpol	2103.00		NIST Webbook
rinpol	2103.00		NIST Webbook
rinpol	2077.00		NIST Webbook
tb	709.97	K	Joback Method
tc	880.96	K	Joback Method
tf	361.05	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.12	J/mol×K	709.97	Joback Method
cpg	937.44	J/mol×K	852.46	Joback Method

cpg	921.48	J/mol×K	823.96	Joback Method
cpg	904.69	J/mol×K	795.46	Joback Method
cpg	887.04	J/mol×K	766.97	Joback Method
cpg	868.53	J/mol×K	738.47	Joback Method
cpg	952.60	J/mol×K	880.96	Joback Method
dvisc	0.0000774	Pa×s	709.97	Joback Method
dvisc	0.0001061	Pa×s	651.82	Joback Method
dvisc	0.0001546	Pa×s	593.66	Joback Method
dvisc	0.0002445	Pa×s	535.51	Joback Method
dvisc	0.0004323	Pa×s	477.36	Joback Method
dvisc	0.0008954	Pa×s	419.20	Joback Method
dvisc	0.0023450	Pa×s	361.05	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=C5129613&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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