Octacosanoic acid, methyl ester

Other names:	Methyl octacosanoate
	Montanic acid, methyl ester
Inchi:	InChI=1S/C29H58O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-2
InchiKey:	ZKHOYAKAFALNQD-UHFFFAOYSA-N
Formula:	C29H58O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	438.77
CAS:	55682-92-3

Physical Properties

Property code	Value	Unit	Source
gf	-40.62	kJ/mol	Joback Method
hf	-886.69	kJ/mol	Joback Method
hfus	73.65	kJ/mol	Joback Method
hvap	157.50 ± 4.50	kJ/mol	NIST Webbook
log10ws	-10.82		Crippen Method
logp	10.322		Crippen Method
mcvol	426.910	ml/mol	McGowan Method
pc	638.98	kPa	Joback Method
rinpol	3115.00		NIST Webbook
rinpol	3140.70		NIST Webbook
rinpol	3115.00		NIST Webbook
rinpol	3112.00		NIST Webbook
rinpol	3108.00		NIST Webbook
rinpol	3112.00		NIST Webbook
rinpol	3116.12		NIST Webbook
rinpol	3144.00		NIST Webbook
rinpol	3140.70		NIST Webbook
rinpol	3125.00		NIST Webbook
tb	939.21	K	Joback Method
tc	1161.87	K	Joback Method
tf	488.75	K	Joback Method
vc	1.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1609.96	J/mol×K	1161.87	Joback Method
cpg	1482.38	J/mol×K	939.21	Joback Method
cpg	1507.73	J/mol×K	976.32	Joback Method
cpg	1531.33	J/mol×K	1013.43	Joback Method
cpg	1553.27	J/mol×K	1050.54	Joback Method
cpg	1573.64	J/mol×K	1087.65	Joback Method
cpg	1592.51	J/mol×K	1124.76	Joback Method
dvisc	0.0000197	Pa×s	939.21	Joback Method
dvisc	0.0005585	Pa×s	488.75	Joback Method
dvisc	0.0002206	Pa×s	563.83	Joback Method
dvisc	0.0001084	Pa×s	638.90	Joback Method
dvisc	0.0000618	Pa×s	713.98	Joback Method
dvisc	0.0000393	Pa×s	789.06	Joback Method
dvisc	0.0000270	Pa×s	864.13	Joback Method
hfust	109.70	kJ/mol	340.20	NIST Webbook

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=C55682923&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
hfust: Enthalpy of fusion at a given temperature
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