Hexacosanoic acid, methyl ester

Other names: 26:0, Me ester
Cerotic acid methyl ester
Methyl hexacosanoate
Inchi: InChI=1S/C27H54O2/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: VHUJBYYFFWDLNM-UHFFFAOYSA-N
Formula: C27H54O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 410.72
CAS: 5802-82-4

Physical Properties

Property code	Value	Unit	Source
gf	-57.46	kJ/mol	Joback Method
hf	-845.41	kJ/mol	Joback Method
hfus	68.47	kJ/mol	Joback Method
hvap	147.10 ± 4.50	kJ/mol	NIST Webbook
log10ws	-9.99		Crippen Method
logp	9.542		Crippen Method
mcvol	398.730	ml/mol	McGowan Method
pc	705.83	kPa	Joback Method
rinpol	2919.00		NIST Webbook
rinpol	2913.00		NIST Webbook
rinpol	2904.00		NIST Webbook
rinpol	2929.20		NIST Webbook
rinpol	2943.00		NIST Webbook
rinpol	2915.05		NIST Webbook
rinpol	2940.00		NIST Webbook
rinpol	2914.00		NIST Webbook
rinpol	2918.00		NIST Webbook
rinpol	2903.00		NIST Webbook
rinpol	477.90		NIST Webbook
rinpol	477.80		NIST Webbook
rinpol	2918.00		NIST Webbook
rinpol	2943.00		NIST Webbook
rinpol	2934.00		NIST Webbook
rinpol	2941.60		NIST Webbook
rinpol	477.90		NIST Webbook

rinpol	2929.20		NIST Webbook
rinpol	2941.60		NIST Webbook
tb	893.45	K	Joback Method
tc	1097.77	K	Joback Method
tf	466.21	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.54	J/mol×K	893.45	Joback Method
cpg	1374.21	J/mol×K	927.50	Joback Method
cpg	1396.42	J/mol×K	961.56	Joback Method
cpg	1417.22	J/mol×K	995.61	Joback Method
cpg	1436.68	J/mol×K	1029.66	Joback Method
cpg	1454.85	J/mol×K	1063.71	Joback Method
cpg	1471.80	J/mol×K	1097.77	Joback Method
dvisc	0.0007281	Pa×s	466.21	Joback Method
dvisc	0.0002915	Pa×s	537.42	Joback Method
dvisc	0.0001446	Pa×s	608.62	Joback Method
dvisc	0.0000831	Pa×s	679.83	Joback Method
dvisc	0.0000530	Pa×s	751.04	Joback Method
dvisc	0.0000366	Pa×s	822.24	Joback Method
dvisc	0.0000268	Pa×s	893.45	Joback Method
hfust	101.30	kJ/mol	336.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	3.49900e+01
Coeff. B	-1.62052e+04
Coeff. C	-1.70222e+02
Temperature range (K), min.	637.20
Temperature range (K), max.	716.25

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=C5802824&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume