Pentacosanoic acid, methyl ester

Other names: methyl pentacosanoate
Inchi: InChI=1S/C26H52O2/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: WOPKHAQDUMDJIY-UHFFFAOYSA-N
Formula: C26H52O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 396.69
CAS: 55373-89-2

Physical Properties

Property code	Value	Unit	Source
gf	-65.88	kJ/mol	Joback Method
hf	-824.77	kJ/mol	Joback Method
hfus	65.88	kJ/mol	Joback Method
hvap	142.00 ± 4.50	kJ/mol	NIST Webbook
log10ws	-9.57		Crippen Method
logp	9.152		Crippen Method
mcvol	384.640	ml/mol	McGowan Method
pc	743.26	kPa	Joback Method
rinpol	2813.00		NIST Webbook
rinpol	464.30		NIST Webbook
rinpol	2822.90		NIST Webbook
rinpol	2813.71		NIST Webbook
rinpol	2817.00		NIST Webbook
rinpol	464.30		NIST Webbook
tb	870.57	K	Joback Method
tc	1067.44	K	Joback Method
tf	454.94	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1403.78	J/mol×K	1067.44	Joback Method
cpg	1285.37	J/mol×K	870.57	Joback Method

cpg	1308.31	J/mol×K	903.38	Joback Method
cpg	1329.90	J/mol×K	936.19	Joback Method
cpg	1350.19	J/mol×K	969.01	Joback Method
cpg	1369.24	J/mol×K	1001.82	Joback Method
cpg	1387.08	J/mol×K	1034.63	Joback Method
dvisc	0.0000311	Pa×s	870.57	Joback Method
dvisc	0.0008279	Pa×s	454.94	Joback Method
dvisc	0.0003338	Pa×s	524.21	Joback Method
dvisc	0.0001664	Pa×s	593.48	Joback Method
dvisc	0.0000959	Pa×s	662.75	Joback Method
dvisc	0.0000614	Pa×s	732.03	Joback Method
dvisc	0.0000424	Pa×s	801.30	Joback Method
hfust	92.00	kJ/mol	332.20	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=C55373892&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