Heptacosanoic acid, methyl ester

Other names: Methyl heptacosanoate
Inchi: InChI=1S/C28H56O2/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: SCVPLVIKFSVDDH-UHFFFAOYSA-N
Formula: C28H56O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 424.74
CAS: 55682-91-2

Physical Properties

Property code	Value	Unit	Source
gf	-49.04	kJ/mol	Joback Method
hf	-866.05	kJ/mol	Joback Method
hfus	71.06	kJ/mol	Joback Method
hvap	152.20 ± 4.50	kJ/mol	NIST Webbook
log10ws	-10.41		Crippen Method
logp	9.932		Crippen Method
mcvol	412.820	ml/mol	McGowan Method
pc	671.16	kPa	Joback Method
rinpol	3014.00		NIST Webbook
rinpol	3027.00		NIST Webbook
rinpol	3015.64		NIST Webbook
rinpol	491.00		NIST Webbook
rinpol	3014.00		NIST Webbook
tb	916.33	K	Joback Method
tc	1129.21	K	Joback Method
tf	477.48	K	Joback Method
vc	1.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1540.54	J/mol×K	1129.21	Joback Method
cpg	1416.23	J/mol×K	916.33	Joback Method
cpg	1440.70	J/mol×K	951.81	Joback Method

cpg	1463.57	J/mol×K	987.29	Joback Method
cpg	1484.93	J/mol×K	1022.77	Joback Method
cpg	1504.83	J/mol×K	1058.25	Joback Method
cpg	1523.34	J/mol×K	1093.73	Joback Method
dvisc	0.0000230	Pa×s	916.33	Joback Method
dvisc	0.0006385	Pa×s	477.48	Joback Method
dvisc	0.0002539	Pa×s	550.62	Joback Method
dvisc	0.0001253	Pa×s	623.76	Joback Method
dvisc	0.0000717	Pa×s	696.90	Joback Method
dvisc	0.0000457	Pa×s	770.05	Joback Method
dvisc	0.0000314	Pa×s	843.19	Joback Method
hfust	100.70	kJ/mol	336.20	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55682912&Units=SI
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

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