17-Octadecynoic acid, methyl ester

Inchi: InChI=1S/C19H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h1H,4-18
InchiKey: RLSBXSWPYYCJIV-UHFFFAOYSA-N
Formula: C19H34O2
SMILES: C#CCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 294.47

Physical Properties

Property code	Value	Unit	Source
gf	98.25	kJ/mol	Joback Method
hf	-388.39	kJ/mol	Joback Method
hfus	50.73	kJ/mol	Joback Method
hvap	66.90	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.644		Crippen Method
mcvol	277.410	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2150.70		NIST Webbook
tb	700.53	K	Joback Method
tc	874.48	K	Joback Method
tf	423.02	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.07	J/mol×K	700.53	Joback Method
cpg	816.36	J/mol×K	729.52	Joback Method
cpg	833.80	J/mol×K	758.51	Joback Method
cpg	850.42	J/mol×K	787.51	Joback Method
cpg	866.23	J/mol×K	816.50	Joback Method
cpg	881.28	J/mol×K	845.49	Joback Method
cpg	895.57	J/mol×K	874.48	Joback Method

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=U333540&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
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