Octadecenoic 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/h7-8,10-
InchiKey: WTTJVINHCBCLGX-ZDVGBALWSA-N
Formula: C19H34O2
SMILES: CCCCCC=CCC=CCCCCCCCC(=O)OC
Mol. weight [g/mol]: 294.47

Physical Properties

Property code	Value	Unit	Source
gf	35.62	kJ/mol	Joback Method
hf	-445.85	kJ/mol	Joback Method
hfus	48.16	kJ/mol	Joback Method
hvap	66.96	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.973		Crippen Method
mcvol	277.410	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2078.00		NIST Webbook
rinpol	2111.00		NIST Webbook
rinpol	357.60		NIST Webbook
rinpol	357.60		NIST Webbook
tb	718.73	K	Joback Method
tc	896.01	K	Joback Method
tf	365.89	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.45	J/mol×K	718.73	Joback Method
cpg	821.70	J/mol×K	748.28	Joback Method
cpg	839.08	J/mol×K	777.82	Joback Method
cpg	855.63	J/mol×K	807.37	Joback Method
cpg	871.40	J/mol×K	836.92	Joback Method
cpg	886.41	J/mol×K	866.47	Joback Method

cpg	900.71	J/mol×K	896.01	Joback Method
dvisc	0.0016090	Pa×s	365.89	Joback Method
dvisc	0.0006439	Pa×s	424.70	Joback Method
dvisc	0.0003219	Pa×s	483.50	Joback Method
dvisc	0.0001871	Pa×s	542.31	Joback Method
dvisc	0.0001209	Pa×s	601.12	Joback Method
dvisc	0.0000845	Pa×s	659.92	Joback Method
dvisc	0.0000626	Pa×s	718.73	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R266652&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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

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