6-Hexadecenoic acid, 7-methyl,methyl ester (Z)

Inchi: InChI=1S/C18H34O2/c1-4-5-6-7-8-9-11-14-17(2)15-12-10-13-16-18(19)20-3/h15H,4-14,1

InchiKey: OQDOMEGWVNDDSV-ICFOKQHNSA-N

Formula: C18H34O2

SMILES: CCCCCCCCCC(C)=CCCCCC(=O)OC

Mol. weight [g/mol]: 282.46

Physical Properties

Property code	Value	Unit	Source
gf	-61.57	kJ/mol	Joback Method
hf	-552.22	kJ/mol	Joback Method
hfus	44.05	kJ/mol	Joback Method
hvap	64.86	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.807		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	1968.00		NIST Webbook
tb	691.57	K	Joback Method
tc	865.71	K	Joback Method
tf	345.74	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.67	J/mol×K	691.57	Joback Method
cpg	786.15	J/mol×K	720.59	Joback Method
cpg	803.78	J/mol×K	749.62	Joback Method
cpg	820.59	J/mol×K	778.64	Joback Method
cpg	836.60	J/mol×K	807.66	Joback Method
cpg	851.84	J/mol×K	836.68	Joback Method
cpg	866.35	J/mol×K	865.71	Joback Method

Sources

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=U245695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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