

2,5-Octadecadiynoic acid, methyl ester

Other names:	2,5-Octadecadiynoic acid, methyl ester
Inchi:	InChI=1S/C19H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h3-13,16
InchiKey:	XQDLQQYTXOVDQQ-UHFFFAOYSA-N
Formula:	C19H30O2
SMILES:	CCCCCCCCCCCC#CCC#CC(=O)OC
Mol. weight [g/mol]:	290.44
CAS:	57156-91-9

Physical Properties

Property code	Value	Unit	Source
gf	280.78	kJ/mol	Joback Method
hf	-135.69	kJ/mol	Joback Method
hfus	54.00	kJ/mol	Joback Method
hvap	71.35	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.867		Crippen Method
mcvol	268.810	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
tb	728.41	K	Joback Method
tc	922.41	K	Joback Method
tf	588.25	K	Joback Method
vc	1.048	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.45	J/molxK	728.41	Joback Method
cpg	777.66	J/molxK	760.74	Joback Method
cpg	794.94	J/molxK	793.08	Joback Method
cpg	811.30	J/molxK	825.41	Joback Method
cpg	826.77	J/molxK	857.74	Joback Method
cpg	841.38	J/molxK	890.08	Joback Method
cpg	855.14	J/molxK	922.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C57156919&Units=SI

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
h vap:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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