10,12-Octadecadiynoic acid

Inchi: InChI=1S/C18H28O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h2-5,10-17H
InchiKey: WNNYSRHBDYRXCH-UHFFFAOYSA-N
Formula: C18H28O2
SMILES: CCCCCC#CC#CCCCCCCCCC(=O)O
Mol. weight [g/mol]: 276.41
CAS: 7333-25-7

Physical Properties

Property code	Value	Unit	Source
gf	240.54	kJ/mol	Joback Method
hf	-135.06	kJ/mol	Joback Method
hfus	54.31	kJ/mol	Joback Method
hvap	83.39	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.779		Crippen Method
mcvol	254.720	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2202.00		NIST Webbook
rinpol	2202.00		NIST Webbook
tb	775.29	K	Joback Method
tc	966.64	K	Joback Method
tf	615.57	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.20	J/mol×K	775.29	Joback Method
cpg	755.68	J/mol×K	807.18	Joback Method
cpg	770.36	J/mol×K	839.07	Joback Method
cpg	784.27	J/mol×K	870.97	Joback Method
cpg	797.45	J/mol×K	902.86	Joback Method
cpg	809.93	J/mol×K	934.75	Joback Method
cpg	821.74	J/mol×K	966.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7333257&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
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