

trans-13-Octadecenoic acid

Inchi:	InChI=1S/C18H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h5-6H,2-4,7
InchiKey:	BDLLSHRIFPDGQB-AATRIKPKSA-N
Formula:	C18H34O2
SMILES:	CCCC=CCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	282.46
CAS:	693-71-0

Physical Properties

Property code	Value	Unit	Source
gf	-84.84	kJ/mol	Joback Method
hf	-562.44	kJ/mol	Joback Method
hfus	48.26	kJ/mol	Joback Method
hvap	79.05	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	6.109		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2163.60		NIST Webbook
rinpol	2163.60		NIST Webbook
tb	761.45	K	Joback Method
tc	937.21	K	Joback Method
tf	398.29	K	Joback Method
vc	1.048	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.35	J/mol×K	761.45	Joback Method
cpg	827.83	J/mol×K	790.74	Joback Method
cpg	843.52	J/mol×K	820.04	Joback Method
cpg	858.48	J/mol×K	849.33	Joback Method
cpg	872.72	J/mol×K	878.62	Joback Method
cpg	886.31	J/mol×K	907.92	Joback Method
cpg	899.26	J/mol×K	937.21	Joback Method

dvisc	0.0023727	Paxs	398.29	Joback Method
dvisc	0.0006419	Paxs	458.82	Joback Method
dvisc	0.0002355	Paxs	519.34	Joback Method
dvisc	0.0001065	Paxs	579.87	Joback Method
dvisc	0.0000560	Paxs	640.40	Joback Method
dvisc	0.0000329	Paxs	700.92	Joback Method
dvisc	0.0000210	Paxs	761.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C693710&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

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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