7,10,13-Hexadecatrienoic acid

Inchi: InChI=1S/C16H26O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h3-4,6-7,9-10H,2,5
InchiKey: KBGYPXOSNDMZRV-IUQGRGSQSA-N
Formula: C16H26O2
SMILES: CCC=CCC=CCC=CCCCCCC(=O)O
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	58.76	kJ/mol	Joback Method
hf	-286.72	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	74.51	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.880		Crippen Method
mcvol	230.840	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	1989.00		NIST Webbook
rinpol	1989.00		NIST Webbook
tb	724.01	K	Joback Method
tc	904.45	K	Joback Method
tf	365.59	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.07	J/mol×K	724.01	Joback Method
cpg	664.43	J/mol×K	754.08	Joback Method
cpg	678.10	J/mol×K	784.16	Joback Method
cpg	691.13	J/mol×K	814.23	Joback Method
cpg	703.59	J/mol×K	844.30	Joback Method
cpg	715.51	J/mol×K	874.38	Joback Method
cpg	726.95	J/mol×K	904.45	Joback Method
dvisc	0.0033563	Pa×s	365.59	Joback Method

dvisc	0.0008065	Pa×s	425.33	Joback Method
dvisc	0.0002754	Pa×s	485.06	Joback Method
dvisc	0.0001190	Pa×s	544.80	Joback Method
dvisc	0.0000607	Pa×s	604.54	Joback Method
dvisc	0.0000349	Pa×s	664.27	Joback Method
dvisc	0.0000220	Pa×s	724.01	Joback Method

Sources

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=R273828&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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