

6-octadecenoic acid

Other names:	Petroselenic 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/h12-13H,2-
InchiKey:	CNVZJPUDSLNTQU-SEYXRHQNSA-N
Formula:	C18H34O2
SMILES:	CCCCCCCCCCCC=CCCCC(=O)O
Mol. weight [g/mol]:	282.46
CAS:	4712-34-9

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	2073.00		NIST Webbook
rinpol	2073.00		NIST Webbook
tb	761.45	K	Joback Method
tc	937.21	K	Joback Method
tf	398.29	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	899.26	J/mol×K	937.21	Joback Method
dvisc	0.0000210	Paxs	761.45	Joback Method
dvisc	0.0000329	Paxs	700.92	Joback Method
dvisc	0.0000560	Paxs	640.40	Joback Method
dvisc	0.0001065	Paxs	579.87	Joback Method
dvisc	0.0002355	Paxs	519.34	Joback Method
dvisc	0.0006419	Paxs	458.82	Joback Method
dvisc	0.0023727	Paxs	398.29	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52924e+01
Coeff. B	-5.81882e+03
Coeff. C	-1.25923e+02
Temperature range (K), min.	514.15
Temperature range (K), max.	709.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4712349&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
pvap:	Vapor 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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