Heptadecanal-

Other names: 1-Heptadecanal
n-Heptadecanal
Inchi: InChI=1S/C17H34O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18/h17H,2-16H2,1H3
InchiKey: PIYDVAYKYBWPPY-UHFFFAOYSA-N
Formula: C17H34O
SMILES: CCCCCCCCCCCCCCCCC=O
Mol. weight [g/mol]: 254.45
CAS: 629-90-3

Physical Properties

Property code	Value	Unit	Source
gf	-7.26	kJ/mol	Joback Method
hf	-479.79	kJ/mol	Joback Method
hfus	42.07	kJ/mol	Joback Method
hvap	60.16	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	6.057		Crippen Method
mcvol	251.960	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
rinpol	1913.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1898.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1903.00		NIST Webbook
rinpol	1922.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1898.00		NIST Webbook

rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1930.00		NIST Webbook
ripol	2249.00		NIST Webbook
ripol	2247.00		NIST Webbook
tb	591.15 ± 4.00	K	NIST Webbook
tc	801.08	K	Joback Method
tf	309.00 ± 4.00	K	NIST Webbook
tf	309.00 ± 4.00	K	NIST Webbook
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.89	J/mol×K	637.02	Joback Method
cpg	718.21	J/mol×K	664.36	Joback Method
cpg	735.75	J/mol×K	691.71	Joback Method
cpg	752.55	J/mol×K	719.05	Joback Method
cpg	768.62	J/mol×K	746.40	Joback Method
cpg	783.98	J/mol×K	773.74	Joback Method
cpg	798.67	J/mol×K	801.08	Joback Method
dvisc	0.0037967	Pa×s	323.35	Joback Method
dvisc	0.0015351	Pa×s	375.63	Joback Method
dvisc	0.0007744	Pa×s	427.91	Joback Method
dvisc	0.0004534	Pa×s	480.19	Joback Method
dvisc	0.0002949	Pa×s	532.46	Joback Method
dvisc	0.0002072	Pa×s	584.74	Joback Method
dvisc	0.0001542	Pa×s	637.02	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C629903&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume