3-Heptadecanone

Inchi: InChI=1S/C17H34O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17(18)4-2/h3-16H2,1-2H3
InchiKey: PXJYBWGEOVYLSM-UHFFFAOYSA-N
Formula: C17H34O
SMILES: CCCCCCCCCCCCCCC(=O)CC
Mol. weight [g/mol]: 254.45
CAS: 84534-29-2

Physical Properties

Property code	Value	Unit	Source
gf	-36.66	kJ/mol	Joback Method
hf	-506.79	kJ/mol	Joback Method
hfus	41.38	kJ/mol	Joback Method
hvap	60.18	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	6.057		Crippen Method
mcvol	251.960	ml/mol	McGowan Method
pc	1287.44	kPa	Joback Method
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1878.00		NIST Webbook
rinpol	1880.00		NIST Webbook
ripol	2155.00		NIST Webbook
ripol	2155.00		NIST Webbook
tb	642.23	K	Joback Method
tc	809.06	K	Joback Method
tf	331.28	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.79	J/mol×K	642.23	Joback Method

cpg	785.94	J/mol×K	781.26	Joback Method
cpg	770.42	J/mol×K	753.45	Joback Method
cpg	754.16	J/mol×K	725.65	Joback Method
cpg	737.15	J/mol×K	697.84	Joback Method
cpg	719.37	J/mol×K	670.04	Joback Method
cpg	800.76	J/mol×K	809.06	Joback Method
dvisc	0.0001395	Pa×s	642.23	Joback Method
dvisc	0.0001873	Pa×s	590.40	Joback Method
dvisc	0.0002662	Pa×s	538.58	Joback Method
dvisc	0.0004078	Pa×s	486.75	Joback Method
dvisc	0.0006915	Pa×s	434.93	Joback Method
dvisc	0.0013527	Pa×s	383.11	Joback Method
dvisc	0.0032643	Pa×s	331.28	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47776e+01
Coeff. B	-4.98789e+03
Coeff. C	-1.04850e+02
Temperature range (K), min.	449.08
Temperature range (K), max.	631.77

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=C84534292&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/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
pvap:	Vapor 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