7-Heptadecanone

Inchi: InChI=1S/C17H34O/c1-3-5-7-9-10-11-12-14-16-17(18)15-13-8-6-4-2/h3-16H2,1-2H3
InchiKey: NFRKSAMCQGIGRC-UHFFFAOYSA-N
Formula: C17H34O
SMILES: CCCCCCCCCCC(=O)CCCCCC
Mol. weight [g/mol]: 254.45
CAS: 6064-42-2

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
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	719.37	J/mol×K	670.04	Joback Method
cpg	737.15	J/mol×K	697.84	Joback Method
cpg	754.16	J/mol×K	725.65	Joback Method
cpg	770.42	J/mol×K	753.45	Joback Method
cpg	785.94	J/mol×K	781.26	Joback Method
cpg	800.76	J/mol×K	809.06	Joback Method
dvisc	0.0032643	Pa×s	331.28	Joback Method
dvisc	0.0013527	Pa×s	383.11	Joback Method

dvisc	0.0006915	Pa×s	434.93	Joback Method
dvisc	0.0004078	Pa×s	486.75	Joback Method
dvisc	0.0002662	Pa×s	538.58	Joback Method
dvisc	0.0001873	Pa×s	590.40	Joback Method
dvisc	0.0001395	Pa×s	642.23	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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C6064422&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume