1-Hepten-3-one

Other names: 1-Heptene-3-one
Inchi: InChI=1S/C7H12O/c1-3-5-6-7(8)4-2/h4H,2-3,5-6H2,1H3
InchiKey: OYLCUJRJCUXQBQ-UHFFFAOYSA-N
Formula: C7H12O
SMILES: C=CC(=O)CCCC
Mol. weight [g/mol]: 112.17
CAS: 2918-13-0

Physical Properties

Property code	Value	Unit	Source
gf	-33.02	kJ/mol	Joback Method
hf	-174.96	kJ/mol	Joback Method
hfus	14.20	kJ/mol	Joback Method
hvap	37.25	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	856.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	876.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1200.00		NIST Webbook
tb	410.11	K	Joback Method
tc	590.38	K	Joback Method
tf	216.82	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	200.30	J/mol×K	410.11	Joback Method
cpg	249.51	J/mol×K	560.33	Joback Method
cpg	240.53	J/mol×K	530.29	Joback Method
cpg	231.14	J/mol×K	500.24	Joback Method
cpg	221.31	J/mol×K	470.20	Joback Method
cpg	211.03	J/mol×K	440.15	Joback Method
cpg	258.07	J/mol×K	590.38	Joback Method
dvisc	0.0002965	Pa×s	410.11	Joback Method
dvisc	0.0003766	Pa×s	377.89	Joback Method
dvisc	0.0005002	Pa×s	345.68	Joback Method
dvisc	0.0007042	Pa×s	313.47	Joback Method
dvisc	0.0010723	Pa×s	281.25	Joback Method
dvisc	0.0018203	Pa×s	249.03	Joback Method
dvisc	0.0036163	Pa×s	216.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37838e+01
Coeff. B	-3.46752e+03
Coeff. C	-5.99520e+01
Temperature range (K), min.	316.88
Temperature range (K), max.	469.23

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2918130&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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