Heptane, 1,1,1,7-tetrachloro-

Other names: 1,1,1,7-Tetrachloroheptane
Inchi: InChI=1S/C7H12Cl4/c8-6-4-2-1-3-5-7(9,10)11/h1-6H2
InchiKey: HIZWVJSDYNNBMS-UHFFFAOYSA-N
Formula: C7H12Cl4
SMILES: ClCCCCCCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 237.98
CAS: 3922-36-9

Physical Properties

Property code	Value	Unit	Source
gf	-36.82	kJ/mol	Joback Method
hf	-259.52	kJ/mol	Joback Method
hfus	23.26	kJ/mol	Joback Method
hvap	47.42	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.546		Crippen Method
mcvol	158.450	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
tb	506.05	K	Joback Method
tc	708.60	K	Joback Method
tf	290.75	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.54	J/mol×K	674.85	Joback Method
cpg	347.02	J/mol×K	641.09	Joback Method
cpg	337.90	J/mol×K	607.33	Joback Method
cpg	328.13	J/mol×K	573.57	Joback Method
cpg	317.68	J/mol×K	539.81	Joback Method
cpg	306.50	J/mol×K	506.05	Joback Method
cpg	363.50	J/mol×K	708.60	Joback Method
dvisc	0.0047299	Pa×s	290.75	Joback Method

dvisc	0.0002953	Pa×s	506.05	Joback Method
dvisc	0.0003931	Pa×s	470.17	Joback Method
dvisc	0.0005485	Pa×s	434.28	Joback Method
dvisc	0.0008126	Pa×s	398.40	Joback Method
dvisc	0.0013013	Pa×s	362.52	Joback Method
dvisc	0.0023111	Pa×s	326.63	Joback Method
hvapt	71.70	kJ/mol	398.50	NIST Webbook
hvapt	69.90	kJ/mol	412.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.18161e+01
Coeff. B	-2.75764e+03
Coeff. C	-1.55163e+02
Temperature range (K), min.	394.37
Temperature range (K), max.	579.12

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=C3922369&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
hvapt:	Enthalpy of vaporization at a given temperature
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