

Heptane, 2-chloro-

Other names:	2-Chloroheptane
Inchi:	InChI=1S/C7H15Cl/c1-3-4-5-6-7(2)8/h7H,3-6H2,1-2H3
InchiKey:	PTSLUOSUHFGQHV-UHFFFAOYSA-N
Formula:	C7H15Cl
SMILES:	CCCCC(C)Cl
Mol. weight [g/mol]:	134.65
CAS:	1001-89-4

Physical Properties

Property code	Value	Unit	Source
gf	-6.31	kJ/mol	Joback Method
hf	-208.83	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	35.17	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.194		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	897.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	894.00		NIST Webbook
ripol	1065.00		NIST Webbook
ripol	1055.00		NIST Webbook
ripol	1077.00		NIST Webbook
ripol	1064.00		NIST Webbook
tb	396.55	K	Joback Method
tc	572.19	K	Joback Method
tf	183.57	K	Joback Method
vc	0.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.17	J/molxK	396.55	Joback Method
cpg	235.16	J/molxK	425.82	Joback Method
cpg	246.67	J/molxK	455.10	Joback Method
cpg	257.72	J/molxK	484.37	Joback Method
cpg	268.31	J/molxK	513.64	Joback Method
cpg	278.47	J/molxK	542.91	Joback Method
cpg	288.19	J/molxK	572.19	Joback Method
dvisc	0.0087444	Paxs	183.57	Joback Method
dvisc	0.0030894	Paxs	219.07	Joback Method
dvisc	0.0014589	Paxs	254.56	Joback Method
dvisc	0.0008278	Paxs	290.06	Joback Method
dvisc	0.0005315	Paxs	325.56	Joback Method
dvisc	0.0003723	Paxs	361.05	Joback Method
dvisc	0.0002780	Paxs	396.55	Joback Method
hvapt	44.80	kJ/mol	368.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48839e+01
Coeff. B	-3.77211e+03
Coeff. C	-5.80910e+01
Temperature range (K), min.	316.52
Temperature range (K), max.	452.15

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1001894&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/ci9903071>

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
hvac:	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
mccvol:	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

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