Octane, 4-chloro-

Other names: 4-Chlorooctane
Inchi: InChI=1S/C8H17Cl/c1-3-5-7-8(9)6-4-2/h8H,3-7H2,1-2H3
InchiKey: SRGMFDQMGOZQPO-UHFFFAOYSA-N
Formula: C8H17Cl
SMILES: CCCCC(Cl)CCC
Mol. weight [g/mol]: 148.67
CAS: 999-07-5

Physical Properties

Property code	Value	Unit	Source
gf	2.11	kJ/mol	Joback Method
hf	-229.47	kJ/mol	Joback Method
hfus	17.15	kJ/mol	Joback Method
hvap	37.40	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.584		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	997.00		NIST Webbook
rinpol	997.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1149.00		NIST Webbook
tb	419.43	K	Joback Method
tc	594.11	K	Joback Method
tf	194.84	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.83	J/mol×K	419.43	Joback Method
cpg	275.97	J/mol×K	448.54	Joback Method
cpg	288.58	J/mol×K	477.66	Joback Method
cpg	300.68	J/mol×K	506.77	Joback Method

cpg	312.27	J/mol×K	535.88	Joback Method
cpg	323.39	J/mol×K	564.99	Joback Method
cpg	334.03	J/mol×K	594.11	Joback Method
dvisc	0.0088497	Pa×s	194.84	Joback Method
dvisc	0.0030882	Pa×s	232.27	Joback Method
dvisc	0.0014434	Pa×s	269.70	Joback Method
dvisc	0.0008121	Pa×s	307.13	Joback Method
dvisc	0.0005177	Pa×s	344.57	Joback Method
dvisc	0.0003605	Pa×s	382.00	Joback Method
dvisc	0.0002677	Pa×s	419.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47709e+01
Coeff. B	-3.92812e+03
Coeff. C	-6.49020e+01
Temperature range (K), min.	336.12
Temperature range (K), max.	480.16

Sources

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

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=C999075&Units=SI

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