Octane, 2-chloro-

Other names: 1-Methylheptyl chloride
2-Chlorooctane
2-Octyl chloride
Inchi: InChI=1S/C8H17Cl/c1-3-4-5-6-7-8(2)9/h8H,3-7H2,1-2H3
InchiKey: HKDCIIMOALDWHF-UHFFFAOYSA-N
Formula: C8H17Cl
SMILES: CCCCCCC(C)Cl
Mol. weight [g/mol]: 148.67
CAS: 628-61-5

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	1006.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1177.00		NIST Webbook
tb	445.05 ± 1.00	K	NIST Webbook
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
hvapt	47.80	kJ/mol	388.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55412e+01
Coeff. B	-4.15231e+03
Coeff. C	-6.49020e+01
Temperature range (K), min.	337.12
Temperature range (K), max.	470.81

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C628615&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

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

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
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