

Octane, 3-chloro-

Other names:	3-Chlorooctane
Inchi:	InChI=1S/C8H17Cl/c1-3-5-6-7-8(9)4-2/h8H,3-7H2,1-2H3
InchiKey:	FYNJWLOOBINARS-UHFFFAOYSA-N
Formula:	C8H17Cl
SMILES:	CCCCC(Cl)CC
Mol. weight [g/mol]:	148.67
CAS:	1117-79-9

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	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
ripol	1166.00		NIST Webbook
tb	419.43	K	Joback Method
tc	594.11	K	Joback Method
tf	194.84	K	Joback Method
vc	0.526	m ³ /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	Paxs	194.84	Joback Method
dvisc	0.0030882	Paxs	232.27	Joback Method
dvisc	0.0014434	Paxs	269.70	Joback Method
dvisc	0.0008121	Paxs	307.13	Joback Method
dvisc	0.0005177	Paxs	344.57	Joback Method
dvisc	0.0003605	Paxs	382.00	Joback Method
dvisc	0.0002677	Paxs	419.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1117799&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
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
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

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