1,8-Dichlorooctane

Other names: Octane, 1,8-dichloro-
Inchi: InChI=1S/C8H16Cl2/c9-7-5-3-1-2-4-6-8-10/h1-8H2
InchiKey: WXYMNDFVLNUAIA-UHFFFAOYSA-N
Formula: C8H16Cl2
SMILES: ClCCCCCCCCCl
Mol. weight [g/mol]: 183.12
CAS: 2162-99-4

Physical Properties

Property code	Value	Unit	Source
gf	-7.38	kJ/mol	Joback Method
hf	-239.93	kJ/mol	Joback Method
hfus	24.87	kJ/mol	Joback Method
hvap	65.60	kJ/mol	NIST Webbook
log10ws	-3.48		Crippen Method
logp	3.805		Crippen Method
mcvol	148.060	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
tb	514.20	K	NIST Webbook
tc	634.68	K	Joback Method
tf	239.76	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.84	J/mol×K	605.12	Joback Method
cpg	338.48	J/mol×K	575.55	Joback Method
cpg	327.65	J/mol×K	545.99	Joback Method
cpg	316.32	J/mol×K	516.43	Joback Method
cpg	304.47	J/mol×K	486.86	Joback Method
cpg	292.09	J/mol×K	457.30	Joback Method

cpg	358.72	J/mol×K	634.68	Joback Method
dvisc	0.0047665	Pa×s	239.76	Joback Method
dvisc	0.0002927	Pa×s	457.30	Joback Method
dvisc	0.0003814	Pa×s	421.04	Joback Method
dvisc	0.0005225	Pa×s	384.79	Joback Method
dvisc	0.0007642	Pa×s	348.53	Joback Method
dvisc	0.0012208	Pa×s	312.27	Joback Method
dvisc	0.0022058	Pa×s	276.02	Joback Method
hvapt	55.90	kJ/mol	460.00	NIST Webbook
hvapt	47.30	kJ/mol	415.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.70	K	1.50	NIST Webbook
tbrp	391.70	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39451e+01
Coeff. B	-4.07901e+03
Coeff. C	-7.68560e+01
Temperature range (K), min.	375.52
Temperature range (K), max.	549.31

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2162994&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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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