1,2-Dichlorooctane

Other names: Octane, 1,2-dichloro
Inchi: InChI=1S/C8H16Cl2/c1-2-3-4-5-6-8(10)7-9/h8H,2-7H2,1H3
InchiKey: LYVLPCUIYWOEBI-UHFFFAOYSA-N
Formula: C8H16Cl2
SMILES: CCCCCCC(Cl)CCl
Mol. weight [g/mol]: 183.12
CAS: 21948-46-9

Physical Properties

Property code	Value	Unit	Source
gf	-9.82	kJ/mol	Joback Method
hf	-245.21	kJ/mol	Joback Method
hfus	21.35	kJ/mol	Joback Method
hvap	57.60	kJ/mol	NIST Webbook
log10ws	-3.59		Crippen Method
logp	3.803		Crippen Method
mcvol	148.060	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
tb	456.86	K	Joback Method
tc	638.13	K	Joback Method
tf	224.76	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.51	J/mol×K	638.13	Joback Method
cpg	350.41	J/mol×K	607.92	Joback Method
cpg	339.83	J/mol×K	577.71	Joback Method
cpg	328.73	J/mol×K	547.49	Joback Method
cpg	317.11	J/mol×K	517.28	Joback Method
cpg	304.94	J/mol×K	487.07	Joback Method
cpg	292.21	J/mol×K	456.86	Joback Method
dvisc	0.0072961	Pa×s	224.76	Joback Method

dvisc	0.0002789	Pa×s	456.86	Joback Method
dvisc	0.0003736	Pa×s	418.18	Joback Method
dvisc	0.0005312	Pa×s	379.49	Joback Method
dvisc	0.0008182	Pa×s	340.81	Joback Method
dvisc	0.0014077	Pa×s	302.13	Joback Method
dvisc	0.0028401	Pa×s	263.44	Joback Method
hvapt	52.00	kJ/mol	430.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43762e+01
Coeff. B	-4.09318e+03
Coeff. C	-7.51880e+01
Temperature range (K), min.	365.72
Temperature range (K), max.	526.74

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21948469&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume