

1,2-DICHLOROOCCTANE

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:	---

Physical Properties

Property code	Value	Unit	Source
af	0.4602		Cheméo Relay (1.0)
gf	-9.82	kJ/mol	Joback Method
hf	-263.75	kJ/mol	Cheméo Relay (1.0)
hfus	21.35	kJ/mol	Joback Method
hvap	55.14	kJ/mol	Cheméo Relay (1.0)
ie	10.26	eV	Cheméo Relay (1.0)
log10ws	-4.66		Cheméo Relay (1.0)
logp	3.803		Crippen Method
mcvol	148.060	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
tb	472.38	K	Cheméo Relay (1.0)
tc	676.18	K	Cheméo Relay (1.0)
tf	249.59	K	Cheméo Relay (1.0)
vc	0.549	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.21	J/mol×K	456.86	Joback Method
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
dvisc	0.0008182	Pa×s	340.81	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	0.0072961	Pa×s	224.76	Joback Method
dvisc	0.0014077	Pa×s	302.13	Joback Method
dvisc	0.0028401	Pa×s	263.44	Joback Method

Correlations

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C21948469&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

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
ie:	Ionization energy
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

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