

1,2-Dibromo-1,1-dichloroethane

Other names:	Ethane, 1,2-dibromo-1,1-dichloro- 1,2-Dibromo-2,2-dichloroethane
Inchi:	InChI=1S/C2H2Br2Cl2/c3-1-2(4,5)6/h1H2
InchiKey:	FIYBYNHDEOSJPL-UHFFFAOYSA-N
Formula:	C2H2Br2Cl2
SMILES:	ClC(Cl)(Br)CBr
Mol. weight [g/mol]:	256.75
CAS:	75-81-0

Physical Properties

Property code	Value	Unit	Source
gf	-26.42	kJ/mol	Joback Method
hf	-72.18	kJ/mol	Joback Method
hfus	12.49	kJ/mol	Joback Method
hvap	40.39	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.908		Crippen Method
mcvol	98.520	ml/mol	McGowan Method
pc	5678.82	kPa	Joback Method
rinpol	1072.00		NIST Webbook
tb	449.11	K	Joback Method
tc	691.70	K	Joback Method
tf	206.30 ± 0.02	K	NIST Webbook
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.35	J/mol×K	449.11	Joback Method
cpg	133.76	J/mol×K	489.54	Joback Method
cpg	137.55	J/mol×K	529.97	Joback Method
cpg	140.79	J/mol×K	570.41	Joback Method
cpg	143.54	J/mol×K	610.84	Joback Method
cpg	145.88	J/mol×K	651.27	Joback Method

cpg	147.86	J/mol×K	691.70	Joback Method
dvisc	0.0035685	Pa×s	294.16	Joback Method
dvisc	0.0022683	Pa×s	319.99	Joback Method
dvisc	0.0015428	Pa×s	345.81	Joback Method
dvisc	0.0011071	Pa×s	371.63	Joback Method
dvisc	0.0008294	Pa×s	397.46	Joback Method
dvisc	0.0006437	Pa×s	423.29	Joback Method
dvisc	0.0005143	Pa×s	449.11	Joback Method
hvapt	45.90	kJ/mol	436.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75810&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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