1,4-Dichlorobenzene-D4

Other names: 1,4-Dichloro-2,3,5,6-tetradeuterobenzene
Benzene, 1,4-dichloro-, [2H4]
Inchi: InChI=1S/C6H4Cl2/c7-5-1-2-6(8)4-3-5/h1-4H/i1D,2D,3D,4D
InchiKey: OCJBOOLMMGQPQU-RHQRLBAQSA-N
Formula: C6D4Cl2
SMILES: Clc1ccc(Cl)cc1
Mol. weight [g/mol]: 151.03
CAS: 3855-82-1

Physical Properties

Property code	Value	Unit	Source
gf	78.56	kJ/mol	Joback Method
hf	26.41	kJ/mol	Joback Method
hfus	13.34	kJ/mol	Joback Method
hvap	40.66	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.993		Crippen Method
mcvol	96.120	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	161.50		NIST Webbook
rinpol	161.50		NIST Webbook
tb	443.20	K	Joback Method
tc	674.86	K	Joback Method
tf	256.16	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.05	J/mol×K	443.20	Joback Method
cpg	157.36	J/mol×K	481.81	Joback Method
cpg	165.09	J/mol×K	520.42	Joback Method
cpg	172.26	J/mol×K	559.03	Joback Method
cpg	178.92	J/mol×K	597.64	Joback Method

cpg	185.08	J/mol×K	636.25	Joback Method
cpg	190.77	J/mol×K	674.86	Joback Method
dvisc	0.0021588	Pa×s	256.16	Joback Method
dvisc	0.0012985	Pa×s	287.33	Joback Method
dvisc	0.0008628	Pa×s	318.51	Joback Method
dvisc	0.0006166	Pa×s	349.68	Joback Method
dvisc	0.0004656	Pa×s	380.85	Joback Method
dvisc	0.0003668	Pa×s	412.03	Joback Method
dvisc	0.0002989	Pa×s	443.20	Joback Method

Sources

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=C3855821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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