

Dichloromethyl radical

Inchi: InChI=1S/CHCl2/c2-1-3/h1H
InchiKey: ZJULYDCRWUEPTK-UHFFFAOYSA-N
Formula: CHCl2
SMILES: Cl[CH]Cl
Mol. weight [g/mol]: 83.92
CAS: 3474-12-2

Physical Properties

Property code	Value	Unit	Source
ea	1.30 ± 0.20	eV	NIST Webbook
ea	1.57 ± 0.14	eV	NIST Webbook
ea	1.52 ± 0.11	eV	NIST Webbook
ea	1.47 ± 0.04	eV	NIST Webbook
gf	-16.38	kJ/mol	Joback Method
hf	-44.92	kJ/mol	Joback Method
hfus	4.90	kJ/mol	Joback Method
hvap	26.05	kJ/mol	Joback Method
ie	8.45	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.54 ± 0.10	eV	NIST Webbook
ie	8.54 ± 0.01	eV	NIST Webbook
ie	8.32 ± 0.01	eV	NIST Webbook
log10ws	-1.15		Crippen Method
logp	1.583		Crippen Method
mvol	47.280	ml/mol	McGowan Method
pc	5602.57	kPa	Joback Method
tb	296.00	K	Joback Method
tc	478.43	K	Joback Method
tf	162.24	K	Joback Method
vc	0.174	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	49.79	J/molxK	296.00	Joback Method
cpg	52.30	J/molxK	326.40	Joback Method
cpg	54.53	J/molxK	356.81	Joback Method
cpg	56.48	J/molxK	387.21	Joback Method
cpg	58.18	J/molxK	417.62	Joback Method
cpg	59.66	J/molxK	448.02	Joback Method
cpg	60.93	J/molxK	478.43	Joback Method
dvisc	0.0007668	Paxs	162.24	Joback Method
dvisc	0.0005993	Paxs	184.53	Joback Method
dvisc	0.0004940	Paxs	206.83	Joback Method
dvisc	0.0004228	Paxs	229.12	Joback Method
dvisc	0.0003719	Paxs	251.41	Joback Method
dvisc	0.0003341	Paxs	273.71	Joback Method
dvisc	0.0003050	Paxs	296.00	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=C3474122&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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