

Dichlorothiolacetic acid

Other names:	«alpha»-Dichlorothioacetic acid
Inchi:	InChI=1S/C2H2Cl2OS/c3-1(4)2(5)6/h1H,(H,5,6)
InchiKey:	FTHIZBAYNLJMRT-UHFFFAOYSA-N
Formula:	C2H2Cl2OS
SMILES:	O=C(S)C(Cl)Cl
Mol. weight [g/mol]:	145.01
CAS:	13639-16-2

Physical Properties

Property code	Value	Unit	Source
gf	-159.87	kJ/mol	Joback Method
hf	-195.47	kJ/mol	Joback Method
hfus	11.45	kJ/mol	Joback Method
hvap	41.91	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.247		Crippen Method
mcvol	81.440	ml/mol	McGowan Method
pc	5495.11	kPa	Joback Method
tb	436.31	K	Joback Method
tc	667.56	K	Joback Method
tf	243.53	K	Joback Method
vc	0.299	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.13	J/mol×K	436.31	Joback Method
cpg	121.31	J/mol×K	474.85	Joback Method
cpg	125.20	J/mol×K	513.39	Joback Method
cpg	128.82	J/mol×K	551.93	Joback Method
cpg	132.18	J/mol×K	590.48	Joback Method
cpg	135.28	J/mol×K	629.02	Joback Method
cpg	138.14	J/mol×K	667.56	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=C13639162&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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