Sulfallate

Other names:	2-Chlorallyl diethyldithiocarbamate
	2-Chloro-2-propene-1-thiol diethyldithiocarbamate
	2-Chloro-2-propenyl diethylcarbamodithioate
	2-Chloroallyl N,N-diethyldithiocarbamate
	2-Chloroallyl diethyldithiocarbamate
	2-Propene-1-thiol, 2-chloro-, diethyldithiocarbamate
	2-chloroprop-2-enyl diethylaminomethanedithioate
	CDEC
	CP 4,742
	CP 4572
	Carbamic acid, diethyldithio-, 2-chloroallyl ester
	Carbamodithioic acid, diethyl-, 2-chloro-2-propenyl ester
	Chlorallyl diethyldithiocarbamate
	Diethylcarbamodithioic acid 2-chloro-2-propenyl ester
	Diethyldithiocarbamic acid 2-chloroallyl ester
	NCI-C00453
	NSC 16085
	Thioallate
	Vegadex
	Vegadex super
	Vegedex
Inchi:	InChI=1S/C8H14ClNS2/c1-4-10(5-2)8(11)12-6-7(3)9/h3-6H2,1-2H3
InchiKey:	XJCLWVXTCRQIDI-UHFFFAOYSA-N
Formula:	C8H14ClNS2
SMILES:	C=C(Cl)CSC(=S)N(CC)CC
Mol. weight [g/mol]:	223.79
CAS:	95-06-7

Physical Properties

Property code	Value	Unit	Source
gf	344.80	kJ/mol	Joback Method
hf	147.35	kJ/mol	Joback Method
hfus	29.84	kJ/mol	Joback Method
hvap	52.79	kJ/mol	Joback Method
log10ws	-3.39		Estimated Solubility Method

log10ws	-3.39		Aqueous Solubility Prediction Method
logp	3.099		Crippen Method
mcvol	169.900	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1704.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1635.00		NIST Webbook
ripol	2390.00		NIST Webbook
tb	567.69	K	Joback Method
tc	788.84	K	Joback Method
tf	295.26	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.40	J/mol×K	567.69	Joback Method
cpg	377.06	J/mol×K	604.55	Joback Method
cpg	388.83	J/mol×K	641.41	Joback Method
cpg	399.78	J/mol×K	678.27	Joback Method
cpg	409.98	J/mol×K	715.12	Joback Method
cpg	419.50	J/mol×K	751.98	Joback Method
cpg	428.41	J/mol×K	788.84	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95067&Units=SI

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