Triallate

Other names: 2,3,3-Trichlorallyl-N,N-(diisopropyl)-thiocarbamat
2,3,3-Trichloroallyl N,N-diisopropylthiocarbamate
2,3,3-Trichloroallyl diisopropylthiocarbamate
2-Propene-1-thiol, 2,3,3-trichloro-, diisopropylcarbamate
Avadex BE
Avadex BW
CP 23426
Carbamic acid, diisopropylthio-, S-(2,3,3-trichloroallyl) ester
Carbamothioic acid, bis(1-methylethyl)-, S-(2,3,3-trichloro-2-propenyl) ester
Carbamothioic acid, bis(isopropyl), S-(2,3,3-trichloroallyl) ester
Diisopropyltrichloroallylthiocarbamate
Dipthal
Far-Go
Far-Go/Avadex BW
N,N-Diisopropyl-2,3,3-trichlorallyl-thiolcarbamate
N-Diisopropylthiocarbamic acid S-2,3,3-trichloro-2-propenyl ester
NSC 379698
S-(2,3,3-Trichloro-2-propenyl) bis(1-methylethyl)carbamothioate
S-(2,3,3-trichloroprop-2-enyl) (di(propan-2-yl)amino)methanethioate
S-2,3,3-Trichloroallyl N,N-diisopropylthiocarbamate
S-2,3,3-Trichloroallyl diisopropylthiocarbamate
Showdown
Thiocarbamic acid, N-diisopropyl-, S-2,3,3-trichloroallyl ester
Triallat
Triamyl

Inchi: InChI=1S/C10H16Cl3NOS/c1-6(2)14(7(3)4)10(15)16-5-8(11)9(12)13/h6-7H,5H2,1-4H3
InchiKey: MWBPRDONLNQCFV-UHFFFAOYSA-N
Formula: C10H16Cl3NOS
SMILES: CC(C)N(C(=O)SCC(Cl)=C(Cl)Cl)C(C)C
Mol. weight [g/mol]: 304.66
CAS: 2303-17-5

Physical Properties

Property code	Value	Unit	Source
gf	70.75	kJ/mol	Joback Method
hf	-213.05	kJ/mol	Joback Method

hfus	33.53	kJ/mol	Joback Method
hvap	65.96	kJ/mol	Joback Method
log10ws	-4.88		Aqueous Solubility Prediction Method
log10ws	-4.88		Estimated Solubility Method
logp	4.844		Crippen Method
mcvol	212.080	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1809.00		NIST Webbook
tb	678.62	K	Joback Method
tc	901.28	K	Joback Method
tf	307.19 ± 0.20	K	NIST Webbook
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.55	J/mol×K	678.62	Joback Method
cpg	510.50	J/mol×K	715.73	Joback Method
cpg	522.54	J/mol×K	752.84	Joback Method
cpg	533.73	J/mol×K	789.95	Joback Method
cpg	544.11	J/mol×K	827.06	Joback Method
cpg	553.76	J/mol×K	864.17	Joback Method
cpg	562.72	J/mol×K	901.28	Joback Method
hfust	27.11	kJ/mol	306.40	NIST Webbook
hsubt	84.00	kJ/mol	305.50	NIST Webbook
hvapt	84.30	kJ/mol	305.50	NIST Webbook

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

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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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