Disulfiram

Other names:

1,1'-Dithiobis(N,N-diethylthioformamide)
Abstensil
Abstinil
Abstinyl
Accel TET
Akrochem TETD
Alcophobin
Alk-Aubs
Ancazide ET
Antabus
Antabuse
Antadix
Antaenyl
Antaethan
Antaethyl
Antaetil
Antalcol
Antetan
Antethyl
Antetil
Anteyl
Anthethyl
Antiaethan
Aversan
Averzan
Bis((diethylamino)thioxomethyl) disulfide
Bis((diethylamino)thioxomethyl)disulphide
Bis(N,N-diethylthiocarbamoyl) disulfide
Bis(N,N-diethylthiocarbamoyl)disulphide
Bis(diethylthiocarbamoyl) disulfide
Bis(diethylthiocarbamoyl)disulphide
Bonibal
Contralin
Contrapot
Cronetal
Dicupral
Disetil
Disulfan
Disulfide, bis(diethylthiocarbamoyl)
Disulfuram

Disulphuram
Dupon 4472
Dupont fungicide 4472
ENT 27,340
Ekagom DTET
Ekagom TEDS
Ekagom TETDS
Ekaland TETD
Ephorran
Espenal
Esperal
Etabus
Ethyl Thiudad
Ethyl Tuads
Ethyl Tuads Rodform
Ethyl Tuex
Ethyl thiram
Ethyl thiurad
Ethyldithiourame
Ethyldithiurame
Exhoran
Exhorran
Formamide, 1,1'-dithiobis(N,N-diethylthio)-
Hoca
Hocakrotenalnci-C02959
Krotenal
N,N,N',N'-Tetraethylthiuram disulfide
N,N,N',N'-Tetraethylthiuram disulphide
NCI-C02959
NSC 190940
Nocbin
Noxal
Perkacit TETD
Perkait TETD
Refusal
Ro-sulfiram
Sanceler TET-G
Soxinol TET
Stopaethyl
Stopetyl
TATD
TETD
TTD

TTS
Tenurid
Tenutex
Tetidis
Tetradin
Tetradine
Tetraethyldithiuram disulfide
Tetraethylthioperoxydicarbonic diamide
Tetraethylthiram disulfide
Tetraethylthiram disulphide
Tetraethylthiuram
Tetraethylthiuram disulfide
Tetraethylthiuram disulphide
Tetraethylthiuram sulfide
Tetraethylthiuran disulfide
Tetraetil
Teturam
Teturamin
Thiocid
Thioperoxydicarbonic diamide ([(H2N)C(S)]2S2), N,N,N',N'-tetraethyl-
Thioperoxydicarbonic diamide, tetraethyl-
Thiosan
Thioscabin
Thireranide
Thiuram E
Thiuram disulfide, tetraethyl-
Thiuranide
Tillram
Tiuram
Tuads, ethyl
USAF B-33
anti-Ethyl
antiCol
antiEtanol
antiEtil
antiKol
antiVitium

Inchi: InChI=1S/C10H20N2S4/c1-5-11(6-2)9(13)15-16-10(14)12(7-3)8-4/h5-8H2,1-4H3
InchiKey: AUZONCFQVSMFAP-UHFFFAOYSA-N
Formula: C10H20N2S4
SMILES: CCN(CC)C(=S)SSC(=S)N(CC)CC
Mol. weight [g/mol]: 296.54
CAS: 97-77-8

Physical Properties

Property code	Value	Unit	Source
gf	555.24	kJ/mol	Joback Method
hf	262.07	kJ/mol	Joback Method
hfus	45.16	kJ/mol	Joback Method
hvap	69.03	kJ/mol	Joback Method
log10ws	-4.72		Aqueous Solubility Prediction Method
log10ws	-3.00		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-4.86		Estimated Solubility Method
logp	3.621		Crippen Method
mcvol	228.520	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	730.72	K	Joback Method
tc	966.00	K	Joback Method
tf	343.77	K	Aqueous Solubility Prediction Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.25	J/mol×K	730.72	Joback Method
cpg	588.89	J/mol×K	769.93	Joback Method
cpg	601.61	J/mol×K	809.15	Joback Method
cpg	613.52	J/mol×K	848.36	Joback Method
cpg	624.75	J/mol×K	887.57	Joback Method
cpg	635.42	J/mol×K	926.79	Joback Method
cpg	645.66	J/mol×K	966.00	Joback Method

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97778&Units=SI
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

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