Phosphorodithioic acid, S-[2-(ethylthio)ethyl] O,O-dimethyl ester

Other names: 2-Ethylthioethyl O,O-dimethyl phosphorodithioate
BAY 23129
BAYER 23129
Compound M-81
Dithiometasystox
Dithiomethon
Dithiometon
Dithiophosphate de O,O-dimethyle et de S-(2-ethylthio-ethyle)
Ekatin
Ekatin ULV
Ekatin aerosol
Ekatine-25
Ethanethiol, 2-(ethylthio)-, S-ester with O,O-dimethyl phosphorodithioate
Intrathion
Intration
Luxistelm
M 81
O,O-Dimethyl S-(2-(ethylthio)ethyl) phosphorodithioate
O,O-Dimethyl S-(2-Ethylthioethyl) dithiophosphate
O,O-Dimethyl-S-(2-aethylthio-aethyl)-dithio phosphat
O,O-Dimethyl-S-(2-ethylmercaptoethyl) dithiophosphate
O,O-Dimethyl-S-(2-ethylthio-ethyl)-dithiofosfaat
O,O-Dimethyl-S-2-ethylmerkaptoethylester kyseliny dithiofosforecne
O,O-Dimetil-S-(etiltio-etil)-ditiofosfato
Phosphorodithioic acid, O,O-dimethyl S-(2-ethylthio)ethyl ester
S-(2-(Ethylthio)ethyl) O,O-dimethylphosphorodithionate
S-(2-(Ethylthio)ethyl)dimethyl phosphorothiolothionate
S-[2-(Ethylthio)ethyl] O,O-dimethyl phosphorodithioate
SAN 230
Thiameton
Thiometon
Veltin

Inchi: InChI=1S/C6H15O2PS3/c1-4-11-5-6-12-9(10,7-2)8-3/h4-6H2,1-3H3

InchiKey: OPASCBHCTNRLRM-UHFFFAOYSA-N

Formula: C6H15O2PS3

SMILES: CCSCCSP(=S)(OC)OC

Mol. weight [g/mol]: 246.36

CAS: 640-15-3

Physical Properties

Property code	Value	Unit	Source
hf	-348.94	kJ/mol	Cheméo Relay (1.0)
hvap	76.80	kJ/mol	NIST Webbook
ie	8.69	eV	Cheméo Relay (1.0)
log10ws	-3.09		Aqueous Solubility Prediction Method
log10ws	-3.09		Estimated Solubility Method
logp	2.990		Crippen Method
mcvol	176.650	ml/mol	McGowan Method
rinpol	1680.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1689.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.86172e+01
Coeff. B	-9.16613e+03
Coeff. C	-1.21000e+00
Temperature range (K), min.	324.76
Temperature range (K), max.	394.51

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C640153&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

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