Aramite

Other names:

Sulfurous acid, 2-chloroethyl 2-[4-(1,1-dimethylethyl)phenoxy]-1-methylethyl ester
Sulfurous acid, 2-(p-tert-butylphenoxy)-1-methylethyl 2-chloroethyl ester
Aramit
Compound 88R
CES
Niagaramite
Ortho-Mite
2-(p-tert-Butylphenoxy)isopropyl 2-chloroethyl sulfite
88R
«beta»-Chloroethyl-«beta»'-(p-tert-butylphenoxy)-«alpha»'-methylethyl sulfite
«beta»-Chloroethyl-«beta»'-(p-t-butylphenoxy)-«alpha»'-methylethyl sulfite
Acaracide
Acrylsaeureaethylester
Aracide
Aramite-15W
Aratron
Ethanol, 2-chloro-, ester with 2-(p-tert-butylphenoxy)-1-methylethyl sulfite
Ethanol, 2-chloro-, 2-(p-tert-butylphenoxy)-1-methylethyl sulfite
ENT 16,519
2-(p-butylphenoxy)-1-methylethyl 2-chloroethyl sulfite
2-(p-t-butylphenoxy)isopropyl 2'-chloroethyl sulfite
2-(p-tert-Butylphenoxy)-1-methylethyl sulfite of 2-chloroethanol
2-(p-tert-Butylphenoxy)-1-methylethyl 2-chloroethyl ester of sulfurous acid
2-(p-tert-Butylphenoxy)-1-methylethyl 2'-chloroethyl sulfite
2-(p-tert-Butylphenoxy)-1-methylethyl-2-choroethyl sulfite
2-(p-tert-Buytlphenoxy)isopropyl 2-chloroethyl sulfite
2-(p-Butylphenoxy)isopropyl 2-chloroethyl sulfite
2-(4-t-butylphenoxy)isopropyl-2-chloroethyl sulphite
2-(4-tert-Butylphenoxy)isopropyl-2-chloroethyl sulfite
2-Chloroethyl sulfite of 1-(p-t-butylphenoxy)-2-propanol
2-Chloroethyl 1-methyl-2-(p-tert-butylphenoxy)ethyl sulfite
2-Propanol, 1-(p-tert-butylphenoxy)-, 2-chloroethyl sulfite
Sulfurous acid, 2-(p-t-butylphenoxy)-1-methylethyl-2-chloroethyl ester
Aramiteararamite-15W
2-(p-terc.Butylfenoxy)isopropyl-2'-chlorethylester kyseliny siricite
Butylphenoxyisopropyl chloroethyl sulfite
2-(4-t-Butylphenoxy)isopropyl-2-chloroethyl sulfite
2-(p-t-Butylphenoxy)isopropyl 2'-chloroethyl sulphite
2-(p-t-Butylphenoxy)-1-methylethyl 2-chloroethyl ester of sulphurous acid
2-(p-t-Butylphenoxy)-1-methylethyl-2-chloroethyl sulfite

2-(p-t-Butylphenoxy)-1-methylethyl 2'-chloroethyl sulphite
2-(p-t-Butylphenoxy)-1-methylethyl sulphite of 2-chloroethanol
2-Chloroethyl 1-methyl-2-(p-t-butylphenoxy)ethyl sulphate
2-Chloroethyl sulphite of 1-(p-t-butylphenoxy)-2-propanol
Ethanol, 2-chloro-, 2-(p-t-butylphenoxy)-1-methylethyl sulfite
2-Propanol, 1-(p-t-butylphenoxy)-, 2-chloroethyl sulfite
2-(p-tert-Butylphenoxy)-1-methylethyl 2-chloroethyl sulfite

Inchi: InChI=1S/C15H23ClO4S/c1-12(20-21(17)19-10-9-16)11-18-14-7-5-13(6-8-14)15(2,3)4/h5

InchiKey: YKFRAOGHWKADFJ-UHFFFAOYSA-N

Formula: C15H23ClO4S

SMILES: CC(COc1ccc(C(C)(C)C)cc1)OS(=O)OCCCl

Mol. weight [g/mol]: 334.86

CAS: 140-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-366.04	kJ/mol	Joback Method
hf	-760.04	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	74.58	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.602		Crippen Method
mcvol	250.520	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	363.69		NIST Webbook
rinpol	363.69		NIST Webbook
rinpol	364.71		NIST Webbook
tb	733.56	K	Joback Method
tc	943.27	K	Joback Method
tf	418.26	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.43	J/mol×K	733.56	Joback Method
cpg	705.80	J/mol×K	768.51	Joback Method

cpg	721.02	J/mol×K	803.46	Joback Method
cpg	735.07	J/mol×K	838.41	Joback Method
cpg	747.98	J/mol×K	873.36	Joback Method
cpg	759.75	J/mol×K	908.31	Joback Method
cpg	770.40	J/mol×K	943.27	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C140578&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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
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