Fenothiocarb

Other names: Carbamothioic acid, N,N-dimethyl-, S-(4-phenoxybutyl) ester
Inchi: InChI=1S/C13H19NO2S/c1-14(2)13(15)17-11-7-6-10-16-12-8-4-3-5-9-12/h3-5,8-9H,6-7,1
InchiKey: HMIBKHHNXANVHR-UHFFFAOYSA-N
Formula: C13H19NO2S
SMILES: CN(C)C(=O)SCCCCOc1ccccc1
Mol. weight [g/mol]: 253.36
CAS: 62850-32-2

Physical Properties

Property code	Value	Unit	Source
gf	80.97	kJ/mol	Joback Method
hf	-210.52	kJ/mol	Joback Method
hfus	33.40	kJ/mol	Joback Method
hvap	64.82	kJ/mol	Joback Method
log10ws	-3.93		Estimated Solubility Method
log10ws	-3.93		Aqueous Solubility Prediction Method
logp	3.260		Crippen Method
mcvol	204.040	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	2136.00		NIST Webbook
rinpol	2136.00		NIST Webbook
tb	681.03	K	Joback Method
tc	896.92	K	Joback Method
tf	313.65	K	Aqueous Solubility Prediction Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.79	J/mol×K	681.03	Joback Method
cpg	554.50	J/mol×K	717.01	Joback Method
cpg	569.15	J/mol×K	752.99	Joback Method

cpg	582.77	J/mol×K	788.97	Joback Method
cpg	595.40	J/mol×K	824.95	Joback Method
cpg	607.05	J/mol×K	860.93	Joback Method
cpg	617.78	J/mol×K	896.92	Joback Method

Sources

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=C62850322&Units=SI

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

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

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