Mcpa-thioethyl

Other names: S-ethyl (4-chloro-2-methylphenoxy)ethanethioate
Inchi: InChI=1S/C11H13ClO2S/c1-3-15-11(13)7-14-10-5-4-9(12)6-8(10)2/h4-6H,3,7H2,1-2H3
InchiKey: AZFKQCNGMSSWDS-UHFFFAOYSA-N
Formula: C11H13ClO2S
SMILES: CCSC(=O)COc1ccc(Cl)cc1C
Mol. weight [g/mol]: 244.74
CAS: 25319-90-8

Physical Properties

Property code	Value	Unit	Source
gf	-77.84	kJ/mol	Joback Method
hf	-275.45	kJ/mol	Joback Method
hfus	28.62	kJ/mol	Joback Method
hvap	64.04	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.307		Crippen Method
mcvol	178.120	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1826.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1826.00		NIST Webbook
tb	670.22	K	Joback Method
tc	902.13	K	Joback Method
tf	401.67	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.08	J/mol×K	670.22	Joback Method
cpg	435.03	J/mol×K	708.87	Joback Method
cpg	447.10	J/mol×K	747.52	Joback Method
cpg	458.30	J/mol×K	786.17	Joback Method
cpg	468.62	J/mol×K	824.83	Joback Method

cpg	478.08	J/mol×K	863.48	Joback Method
cpg	486.67	J/mol×K	902.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25319908&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