Carbamothioic acid, S-[2-oxo-2-(phenylamino)ethyl] ester

Other names: Acetamide, N-phenyl-2-(carbamoylthio)-
Acetanilide, 2-(thiocarbamyl)-
Carbamic acid, thio-, S-ester with 2-mercaptoacetanilide
Carbaminothioglycolic acid anilide
NSC 13336
S-[2-oxo-2-(phenylamino)ethyl] aminomethanethioate
USAF uctl-1766
alpha-Mercaptoacetanilide carbamate
«alpha»-(Thiocarbamyl) acetanilide
Â«alphaÂ»-(Thiocarbamyl) acetanilide

Inchi: InChI=1S/C9H10N2O2S/c10-9(13)14-6-8(12)11-7-4-2-1-3-5-7/h1-5H,6H2,(H2,10,13)(H,1

InchiKey: CEINNGQDMFZTJK-UHFFFAOYSA-N

Formula: C9H10N2O2S

SMILES: NC(=O)SCC(=O)Nc1ccccc1

Mol. weight [g/mol]: 210.25

CAS: 5428-95-5

Physical Properties

Property code	Value	Unit	Source
gf	68.43	kJ/mol	Joback Method
hf	-88.59	kJ/mol	Joback Method
hfus	30.73	kJ/mol	Joback Method
hvap	75.29	kJ/mol	Joback Method
log10ws	-1.32		Aqueous Solubility Prediction Method
logp	1.437		Crippen Method
mcvol	153.360	ml/mol	McGowan Method
pc	4227.54	kPa	Joback Method
tb	731.22	K	Joback Method
tc	980.54	K	Joback Method
tf	487.79	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.18	J/mol×K	731.22	Joback Method
cpg	401.66	J/mol×K	772.77	Joback Method
cpg	411.16	J/mol×K	814.33	Joback Method
cpg	419.70	J/mol×K	855.88	Joback Method
cpg	427.35	J/mol×K	897.43	Joback Method
cpg	434.13	J/mol×K	938.99	Joback Method
cpg	440.09	J/mol×K	980.54	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5428955&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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