

2-Mercaptoacetanilide

Other names:	Thioglycolanilide Thioglycolylanilide Acetamide, 2-mercapto-N-phenyl- Acetanilide, «alpha»-mercapto- Acetanilide, 2-mercapto- N-Phenyl-2-mercaptoacetamide Thioglycolic acid anilide USAF EK-6583 «alpha»-Mercaptoacetanilide alpha-Mercaptoacetanilide NSC 2126
Inchi:	InChI=1S/C8H9NOS/c10-8(6-11)9-7-4-2-1-3-5-7/h1-5,11H,6H2,(H,9,10)
InchiKey:	DLVKRCGYGJZXFK-UHFFFAOYSA-N
Formula:	C8H9NOS
SMILES:	O=C(CS)Nc1ccccc1
Mol. weight [g/mol]:	167.23
CAS:	4822-44-0

Physical Properties

Property code	Value	Unit	Source
gf	118.75	kJ/mol	Joback Method
hf	7.45	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	55.60	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.555		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
tb	576.02	K	Joback Method
tc	819.65	K	Joback Method
tf	345.39	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.83	J/mol×K	576.02	Joback Method
cpg	290.79	J/mol×K	616.62	Joback Method
cpg	301.83	J/mol×K	657.23	Joback Method
cpg	311.99	J/mol×K	697.83	Joback Method
cpg	321.33	J/mol×K	738.44	Joback Method
cpg	329.89	J/mol×K	779.04	Joback Method
cpg	337.71	J/mol×K	819.65	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4822440&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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