

Anthranilic acid, n-[(2-chloroethyl)nitrosocarbamoyl]-

Inchi: InChI=1S/C10H10ClN3O4/c11-5-6-14(13-18)10(17)12-8-4-2-1-3-7(8)9(15)16/h1-4H,5-6H
InchiKey: IRVKQMQRPAWVDV-UHFFFAOYSA-N
Formula: C10H10ClN3O4
SMILES: O=NN(CCCI)C(=O)Nc1cccc1C(=O)O
Mol. weight [g/mol]: 271.66
CAS: 13909-23-4

Physical Properties

Property code	Value	Unit	Source
hf	-464.99	kJ/mol	Joback Method
hvap	92.92	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.139		Crippen Method
mcpvol	180.760	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	823.22	K	Joback Method
tc	1031.38	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13909234&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation 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

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