

2,5-Pyrrolidinedione, 1-bromo-

Other names:	Bromosuccinimide N-Bromosuccinimide NBS Succinbromimide Succinimide, N-bromo- 1-Bromo-2,5-pyrrolidine-dione Succinbromide Succinibromimide N-Bromsuccinimide NSC 16
Inchi:	InChI=1S/C4H4BrNO2/c5-6-3(7)1-2-4(6)8/h1-2H2
InchiKey:	PCLIMKBDDGJMGD-UHFFFAOYSA-N
Formula:	C4H4BrNO2
SMILES:	O=C1CCC(=O)N1Br
Mol. weight [g/mol]:	177.98
CAS:	128-08-5

Physical Properties

Property code	Value	Unit	Source
hfs	-335.90 ± 0.63	kJ/mol	NIST Webbook
ie	10.12	eV	NIST Webbook
ie	10.12	eV	NIST Webbook
log10ws	-0.93		Crippen Method
logp	0.445		Crippen Method
mvol	86.980	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C128085&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfs:	Solid phase enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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