

N-HYDROXYBENZENESULFONAMIDE

Inchi: InChI=1S/C6H7NO3S/c8-7-11(9,10)6-4-2-1-3-5-6/h1-5,8H,(H,7,9,10)
InchiKey: BRMDATNYMUMZLN-UHFFFAOYSA-N
Formula: C6H7NO3S
SMILES: O=S(O)(=NO)c1ccccc1
Mol. weight [g/mol]: 173.19

Physical Properties

Property code	Value	Unit	Source
hf	-245.63	kJ/mol	Cheméo Relay (1.0)
ie	9.84	eV	Cheméo Relay (1.0)
log10ws	-0.65		Cheméo Relay (1.0)
logp	1.376		Crippen Method
mcvol	115.580	ml/mol	McGowan Method
tb	565.82	K	Cheméo Relay (1.0)
tf	429.37	K	Cheméo Relay (1.0)

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C599713&Units=SI>
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

hf: 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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