

1-Aminocyclopropanecarboxylic acid, N-dimethylaminomethylene-

Inchi: InChI=1S/C7H12N2O2/c1-9(2)5-8-7(3-4-7)6(10)11/h5H,3-4H2,1-2H3,(H,10,11)
InchiKey: PBLKPNVCRDIRDP-UHFFFAOYSA-N
Formula: C7H12N2O2
SMILES: CN(C)C=NC1(C(=O)O)CC1
Mol. weight [g/mol]: 156.18

Physical Properties

Property code	Value	Unit	Source
hf	-214.83	kJ/mol	Joback Method
hvap	58.72	kJ/mol	Joback Method
log10ws	-0.09		Crippen Method
logp	0.193		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
rinsol	1517.00		NIST Webbook
rinsol	1517.00		NIST Webbook
tb	601.71	K	Joback Method
tc	804.65	K	Joback Method

Sources

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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375508&Units=SI>

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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