Carmustine

Inchi: InChI=1S/C5H9Cl2N3O2/c6-1-3-8-5(11)10(9-12)4-2-7/h1-4H2,(H,8,11)
InchiKey: DLGOEMSEDOSKAD-UHFFFAOYSA-N
Formula: C5H9Cl2N3O2
SMILES: O=NN(CCCl)C(=O)NCCCl
Mol. weight [g/mol]: 214.05
CAS: 154-93-8

Physical Properties

Property code	Value	Unit	Source
logp	1.157		Crippen Method
mcvol	138.870	ml/mol	McGowan Method
tf	304.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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):
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Latest version available from:

https://www.chemeo.com/cid/110-952-2/Carmustine.pdf

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