Lomustine

Inchi: InChI=1S/C9H16ClN3O2/c10-6-7-13(12-15)9(14)11-8-4-2-1-3-5-8/h8H,1-7H2,(H,11,14)
InchiKey: GQYIWUVLTXOXAJ-UHFFFAOYSA-N
Formula: C9H16ClN3O2
SMILES: O=NN(CCCl)C(=O)NC1CCCCC1
Mol. weight [g/mol]: 233.70
CAS: 13010-47-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Cheméo Relay (1.0)
logp	2.251		Crippen Method
mcvol	172.130	ml/mol	McGowan Method
tf	363.15	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

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Latest version available from:
https://www.chemeo.com/cid/107-804-0/Lomustine.pdf
Generated by Cheméo on 2026-11-08 17:26:09.097627403 +0000 UTC m=+85091.606864069.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.