N-(Cyclohexylthio)phthalimide

Inchi: InChI=1S/C14H15NO2S/c16-13-11-8-4-5-9-12(11)14(17)15(13)18-10-6-2-1-3-7-10/h4-5,
InchiKey: UEZWYKZHXASYJN-UHFFFAOYSA-N
Formula: C14H15NO2S
SMILES: O=C1c2ccccc2C(=O)N1SC1CCCCC1
Mol. weight [g/mol]: 261.35
CAS: 17796-82-6

Physical Properties

Property code	Value	Unit	Source
logp	3.264		Crippen Method
mcvol	192.110	ml/mol	McGowan Method
tf	365.75	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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):
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

Legend

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

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https://www.chemeo.com/cid/107-893-2/N-Cyclohexylthio-phthalimide.pdf

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