

Suprofen

Inchi:	InChI=1S/C14H12O3S/c1-9(14(16)17)10-4-6-11(7-5-10)13(15)12-3-2-8-18-12/h2-9H,1H3
InchiKey:	MDKGKXOCJGEUJW-UHFFFAOYSA-N
Formula:	C14H12O3S
SMILES:	CC(C(=O)O)c1ccc(C(=O)c2cccs2)cc1
Mol. weight [g/mol]:	260.31
CAS:	40828-46-4

Physical Properties

Property code	Value	Unit	Source
hvap	106.17	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
log10ws	-3.10		Cheméo Relay (1.0)
logp	3.167		Crippen Method
mcvol	190.260	ml/mol	McGowan Method
tb	633.87	K	Cheméo Relay (1.0)
tf	397.45	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_Dataset/1031637
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hvap:	Enthalpy of vaporization 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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