

Sulisobenzone

Inchi: InChI=1S/C14H12O6S/c1-20-12-8-11(15)10(7-13(12)21(17,18)19)14(16)9-5-3-2-4-6-9/h2
InchiKey: CXVGEDCSTKKODG-UHFFFAOYSA-N
Formula: C14H12O6S
SMILES: COc1cc(O)c(C(=O)c2ccccc2)cc1S(=O)(=O)O
Mol. weight [g/mol]: 308.31
CAS: 4065-45-6

Physical Properties

Property code	Value	Unit	Source
hfus	43.36	kJ/mol	Joback Method
log10ws	-1.97		Cheméo Relay (1.0)
logp	1.879		Crippen Method
mcvol	207.870	ml/mol	McGowan Method
tb	678.84		Cheméo Relay (1.0)
tf	418.15		Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	1.34200e+01
Coeff. B	1.18801e+00
Coeff. C	-7.57580e-04
Coeff. D	1.72460e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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_Dataset/1031637

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
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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