

Chlorosulfona

Inchi:	InChI=1S/C2Cl6O2S/c3-1(4,5)11(9,10)2(6,7)8
InchiKey:	YBNLWIZAWPBUKQ-UHFFFAOYSA-N
Formula:	C2Cl6O2S
SMILES:	O=S(=O)(C(Cl)(Cl)Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	300.80
CAS:	3064-70-8

Physical Properties

Property code	Value	Unit	Source
hfus	22.67	kJ/mol	Joback Method
logp	3.057		Crippen Method
mcvol	140.570	ml/mol	McGowan Method
tf	310.15	K	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	6.27100e+01
Coeff. B	5.19790e-01
Coeff. C	-4.85400e-04
Coeff. D	1.47200e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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<https://www.chemeo.com/cid/111-143-9/Chlorosulfona.pdf>

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