

Haloprogin

Inchi:	InChI=1S/C9H4Cl3IO/c10-6-4-8(12)9(5-7(6)11)14-3-1-2-13/h4-5H,3H2
InchiKey:	CTETYYAZBPJBHE-UHFFFAOYSA-N
Formula:	C9H4Cl3IO
SMILES:	Clc1cc(Cl)c(OCC#Cl)cc1Cl
Mol. weight [g/mol]:	361.39
CAS:	777-11-7

Physical Properties

Property code	Value	Unit	Source
hfus	33.25	kJ/mol	Joback Method
log10ws	-5.69		Cheméo Relay (1.0)
logp	4.421		Crippen Method
mcvol	173.720	ml/mol	McGowan Method
tf	386.65	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	9.71210e+01
Coeff. B	4.47800e-01
Coeff. C	-2.35340e-04
Coeff. D	3.77800e-08
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
tf:	Normal melting (fusion) point

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