3,6-Dichlorodibenzofuran

Other names: 3,6-dichlorodibenzofuran
Inchi: InChI=1S/C12H6Cl2O/c13-7-4-5-8-9-2-1-3-10(14)12(9)15-11(8)6-7/h1-6H
InchiKey: DMOBGFAKTSXOHG-UHFFFAOYSA-N
Formula: C12H6Cl2O
SMILES: Clc1ccc2c(c1)oc1c(Cl)cccc12
Mol. weight [g/mol]: 237.08
CAS: 74918-40-4

Physical Properties

Property code	Value	Unit	Source
hvap	87.25	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.61		Cheméo Relay (1.0)
logp	4.893		Crippen Method
mcvol	151.910	ml/mol	McGowan Method
tf	461.20 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	32.40	kJ/mol	461.20	NIST Webbook
hsubt	110.90	kJ/mol	339.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74918404&Units=SI
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):

Legend

hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization 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