

2,4-Dichlorophenoxyacetonitrile

Inchi:	InChI=1S/C8H5Cl2NO/c9-6-1-2-8(7(10)5-6)12-4-3-11/h1-2,5H,4H2
InchiKey:	QSDMPLNZSJLFRM-UHFFFAOYSA-N
Formula:	C8H5Cl2NO
SMILES:	N#CCOc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	202.04
CAS:	3956-63-6

Physical Properties

Property code	Value	Unit	Source
gf	113.95	kJ/mol	Joback Method
hf	6.32	kJ/mol	Joback Method
hfus	20.83	kJ/mol	Joback Method
hvap	58.66	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.896		Crippen Method
mcvol	131.550	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
tb	618.44	K	Joback Method
tc	857.15	K	Joback Method
tf	378.44	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.20	J/mol×K	618.44	Joback Method
cpg	270.43	J/mol×K	658.22	Joback Method
cpg	278.10	J/mol×K	698.01	Joback Method
cpg	285.22	J/mol×K	737.79	Joback Method
cpg	291.81	J/mol×K	777.58	Joback Method
cpg	297.86	J/mol×K	817.36	Joback Method
cpg	303.39	J/mol×K	857.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3956636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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