

Benzylideneimine, 2,4-dichloro-n-methyl-

Inchi: InChI=1S/C8H7Cl2N/c1-11-5-6-2-3-7(9)4-8(6)10/h2-5H,1H3
InchiKey: KBMUDWSXRZZNGJ-UHFFFAOYSA-N
Formula: C8H7Cl2N
SMILES: CN=Cc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 188.05
CAS: 17972-00-8

Physical Properties

Property code	Value	Unit	Source
hf	55.88	kJ/mol	Joback Method
hvac	49.09	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	3.042		Crippen Method
mcvol	129.980	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
tb	570.62	K	Joback Method
tc	814.96	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17972008&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions
hvac: 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

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