

3-Amino-2,5-dichlorobenzoic acid, N-dimethylaminomethylene-, methyl ester

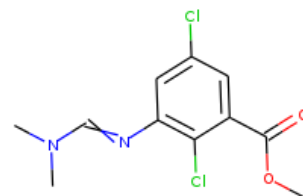
InChI: InChI=1S/C11H12Cl2N2O2/c1-15(2)6-14-9-5-7(12)4-8(10(9)13)11(16)17-3/h4-6H,1-3H3

InChI Key: HYZFQWSMJIFMQX-UHFFFAOYSA-N

Formula: C11H12Cl2N2O2

SMILES: COC(=O)c1cc(Cl)cc(N=CN(C)C)c1Cl

Molecular Weight: 275.13



Physical Properties

Property	Value	Unit	Source
$\Delta_f H^\circ_{\text{gas}}$	-194.78	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	67.62	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.00		Crippen Method
P_c	2218.71	kPa	Joback Method
T_{boil}	732.97	K	Joback Method
T_c	962.73	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H12Cl2N2O2/c1-15\(2\)6-14-9-5-7\(12\)4-8\(10\(9\)13\)11\(16\)17-3/h4-6H,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H12Cl2N2O2/c1-15(2)6-14-9-5-7(12)4-8(10(9)13)11(16)17-3/h4-6H,1-3H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).
 T_{c} : Critical Temperature (K).

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