

1,3,5-Triazin-2-amine, 4,6-dichloro-N-(2-chlorophenyl)-

Other names:

1,3,5-Triazin-2-amine, 4,6-dichloro-N-(2-chlorophenyl)-
s-Triazine, 2,4-dichloro-6-(o-chloroanilino)-
Anilazin
B-622
Bortrysan
Dyrene
Dyrene 50W
Kemate
Triazin
Triazine
Triazine (Pesticide)
Zinochlor
2,4-Dichloro-6-(o-chloroanilino)-s-triazine
Direz
ENT 26,058
NCI-C08684
Triasym
Triasyn
2,4-Dichloro-6-(o-chloroanilino)-s-triazine
2,4-Dichloro-6-(2-chloroanilino)-1,3,5-triazine
4,6-Dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine
2-(2-Chloroanilin)-4,6-dichlor-1,3,5-triazin
(o-Chloroanilino)dichlorotriazine
Aniyaline
Dairene
Dairin
NSC 3851
Dyrene Flussig

Inchi:

InChI=1S/C9H5Cl3N4/c10-5-3-1-2-4-6(5)13-9-15-7(11)14-8(12)16-9/h1-4H,(H,13,14,15,16)

InchiKey:

IMHBYKMAHXWHRP-UHFFFAOYSA-N

Formula:

C9H5Cl3N4

SMILES:

Clc1nc(Cl)nc(Nc2ccccc2Cl)n1

Mol. weight [g/mol]:

275.53

Physical Properties

Property code	Value	Unit	Source
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ie	8.71	eV	Cheméo Relay (1.0)
logp	3.575		Crippen Method
mcvol	166.790	ml/mol	McGowan Method
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	1978.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
tb	597.13	K	Cheméo Relay (1.0)
tf	432.48 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	31.48	kJ/mol	431.00	NIST Webbook
hfust	31.48	kJ/mol	431.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101053&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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