

2-CHLORO-2',6'-ACETOXYLIDIDE

Other names:	N-Chloroacetyl-2,6-dimethylaniline Acetamide, 2-chloro-N-(2,6-dimethylphenyl)- Chloroaceto-2,6-xylidide 1-Chloroacetylamino-2,6-dimethylbenzene 2-Chloro-N-(2,6-dimethylphenyl)acetamide 2-Chloro-2',6'-dimethylacetanilide 2-Chloroaceto-2,6-xylidide 2',6'-Acetoxylidide, 2-chloro- Chloroacet-2,6-xylidide Chloroacetamido-2,6-xylidine NSC 37260
Inchi:	InChI=1S/C10H12ClNO/c1-7-4-3-5-8(2)10(7)12-9(13)6-11/h3-5H,6H2,1-2H3,(H,12,13)
InchiKey:	FPQQSNUTBWFFLB-UHFFFAOYSA-N
Formula:	C10H12ClNO
SMILES:	Cc1cccc(C)c1NC(=O)CCl
Mol. weight [g/mol]:	197.67

Physical Properties

Property code	Value	Unit	Source
hfus	25.81	kJ/mol	Joback Method
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-2.20		Cheméo Relay (1.0)
logp	2.481		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
tf	369.08	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.25	J/mol×K	606.31	Joback Method
cpg	360.66	J/mol×K	643.16	Joback Method
cpg	372.29	J/mol×K	680.02	Joback Method
cpg	383.17	J/mol×K	716.87	Joback Method
cpg	393.33	J/mol×K	753.72	Joback Method

cpg	402.80	J/mol×K	790.58	Joback Method
cpg	411.60	J/mol×K	827.43	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1131017&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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