2-CHLORO-4'-METHOXYACETANILIDE

Other names: 2-Chloro-p-acetanisidide
Acetamide, 2-chloro-N-(4-methoxyphenyl)-
Acetamide, N-(4-methoxyphenyl)-2-chloro-
N-(Chloroacetyl)-p-anisidide
p-Acetanisidide, 2-chloro-

Inchi: InChI=1S/C9H10ClNO2/c1-13-8-4-2-7(3-5-8)11-9(12)6-10/h2-5H,6H2,1H3,(H,11,12)

InchiKey: RLUUKMWWYRMCPY-UHFFFAOYSA-N

Formula: C9H10ClNO2

SMILES: COc1ccc(NC(=O)CCl)cc1

Mol. weight [g/mol]: 199.64

Physical Properties

Property code	Value	Unit	Source
hf	-304.08	kJ/mol	Cheméo Relay (1.0)
hfus	24.80	kJ/mol	Joback Method
hvap	72.17	kJ/mol	Cheméo Relay (1.0)
ie	7.95	eV	Cheméo Relay (1.0)
log10ws	-2.33		Cheméo Relay (1.0)
logp	1.872		Crippen Method
mcvol	143.570	ml/mol	McGowan Method
tb	592.94	K	Cheméo Relay (1.0)
tf	387.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.59	J/mol×K	600.87	Joback Method
cpg	337.21	J/mol×K	637.76	Joback Method
cpg	348.09	J/mol×K	674.66	Joback Method
cpg	358.25	J/mol×K	711.55	Joback Method
cpg	367.72	J/mol×K	748.44	Joback Method
cpg	376.50	J/mol×K	785.34	Joback Method
cpg	384.60	J/mol×K	822.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22303362&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

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