

Acetamide, 2-chloro-N-(2,5-dimethoxyphenyl)-

Other names:	Acetanilide, 2-chloro-2',5'-dimethoxy- 2-Chloro-2',5'-dimethoxyacetanilide 2',5'-Dimethoxy-2-chloroacetanilide 2-Chloro-N-(2,5-dimethoxyphenyl)acetamide Acetamide, N-(2,5-dimethoxyphenyl)-2-chloro-
Inchi:	InChI=1S/C10H12ClNO3/c1-14-7-3-4-9(15-2)8(5-7)12-10(13)6-11/h3-5H,6H2,1-2H3,(H,1
InchiKey:	BDDQUHPZDJEQRL-UHFFFAOYSA-N
Formula:	C10H12ClNO3
SMILES:	COc1ccc(OC)c(NC(=O)CCl)c1
Mol. weight [g/mol]:	229.66
CAS:	22158-78-7

Physical Properties

Property code	Value	Unit	Source
gf	-134.99	kJ/mol	Joback Method
hf	-375.43	kJ/mol	Joback Method
hfus	28.19	kJ/mol	Joback Method
hvap	63.84	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.881		Crippen Method
mcvol	163.530	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1817.00		NIST Webbook
rinpol	1817.00		NIST Webbook
tb	651.15	K	Joback Method
tc	866.91	K	Joback Method
tf	430.89	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.81	J/molxK	651.15	Joback Method
cpg	407.85	J/molxK	687.11	Joback Method

cpg	419.17	J/mol×K	723.07	Joback Method
cpg	429.77	J/mol×K	759.03	Joback Method
cpg	439.64	J/mol×K	794.99	Joback Method
cpg	448.78	J/mol×K	830.95	Joback Method
cpg	457.18	J/mol×K	866.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22158787&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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