

Acetamide, N-(4-methoxyphenyl)-2,2-dichloro-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C9H9Cl2NO2/c1-14-7-4-2-6(3-5-7)12-9(13)8(10)11/h2-5,8H,1H3,(H,12,13)

IKDULUPZZPGFFJ-UHFFFAOYSA-N

C9H9Cl2NO2

COc1ccc(NC(=O)C(Cl)Cl)cc1

234.08

Physical Properties

Property code	Value	Unit	Source
gf	-43.15	kJ/mol	Joback Method
hf	-232.12	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	62.54	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.437		Crippen Method
mcvol	155.810	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
rinpol	1776.00		NIST Webbook
rinpol	1776.00		NIST Webbook
tb	637.86	K	Joback Method
tc	867.35	K	Joback Method
tf	399.79	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.15	J/mol×K	637.86	Joback Method
cpg	360.14	J/mol×K	676.11	Joback Method
cpg	370.34	J/mol×K	714.36	Joback Method
cpg	379.77	J/mol×K	752.61	Joback Method
cpg	388.45	J/mol×K	790.86	Joback Method
cpg	396.40	J/mol×K	829.10	Joback Method
cpg	403.64	J/mol×K	867.35	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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