

2-Propenamide, N-(3,4-dichlorophenyl)-2-methyl-

Other names:	Acrylanilide, 3',4'-dichloro-2-methyl-Dicryl DCMA Methacrylic Acid 3,4-dichloroanilide N 4,556 N-(3,4-Dichlorophenyl)Methacrylamide Niagara 4556 3',4'-Dichloro-2-methylacrylanilide Chloranocryl 3,4-Dichloranilid kyseliny methakrylove 3',4'-Dichloro-2-methacrylanilide N-(3,4-Dichlorophenyl)-2-methyl-2-propenamide FMC 4556 «alpha»-Methylacrylic acid, 3,4-dichloroanilide NIA 4556 Licryl
Inchi:	InChI=1S/C10H9Cl2NO/c1-6(2)10(14)13-7-3-4-8(11)9(12)5-7/h3-5H,1H2,2H3,(H,13,14)
InchiKey:	VCBRBUKGTWLJOB-UHFFFAOYSA-N
Formula:	C10H9Cl2NO
SMILES:	<chem>C=C(C)C(=O)Nc1ccc(Cl)c(Cl)c1</chem>
Mol. weight [g/mol]:	230.09
CAS:	2164-09-2

Physical Properties

Property code	Value	Unit	Source
gf	142.37	kJ/mol	Joback Method
hf	-11.09	kJ/mol	Joback Method
hfus	27.42	kJ/mol	Joback Method
hvap	62.82	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.508		Crippen Method
mcvol	159.730	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	640.30	K	Joback Method
tc	873.47	K	Joback Method
tf	395.70 ± 0.20	K	NIST Webbook
tf	396.06 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.11	J/mol×K	640.30	Joback Method
cpg	360.99	J/mol×K	679.16	Joback Method
cpg	371.08	J/mol×K	718.02	Joback Method
cpg	380.40	J/mol×K	756.88	Joback Method
cpg	389.02	J/mol×K	795.75	Joback Method
cpg	396.97	J/mol×K	834.61	Joback Method
cpg	404.28	J/mol×K	873.47	Joback Method
hfust	32.04	kJ/mol	395.50	NIST Webbook
hfust	32.04	kJ/mol	395.50	NIST Webbook
sfust	80.36	J/mol×K	395.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2164092&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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