

Chloroacetamide, N-ethyl-N-(3-methylphenyl)-

Inchi:	InChI=1S/C11H14ClNO/c1-3-13(11(14)8-12)10-6-4-5-9(2)7-10/h4-7H,3,8H2,1-2H3
InchiKey:	HDVSUKKVAMUTGV-UHFFFAOYSA-N
Formula:	C11H14ClNO
SMILES:	CCN(C(=O)CC)c1cccc(C)c1
Mol. weight [g/mol]:	211.69

Physical Properties

Property code	Value	Unit	Source
gf	114.45	kJ/mol	Joback Method
hf	-106.10	kJ/mol	Joback Method
hfus	26.71	kJ/mol	Joback Method
hvap	56.19	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.587		Crippen Method
mvol	165.880	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1616.00		NIST Webbook
tb	586.48	K	Joback Method
tc	800.24	K	Joback Method
tf	364.99	K	Joback Method
vc	0.617	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.21	J/mol×K	586.48	Joback Method
cpg	398.34	J/mol×K	622.11	Joback Method
cpg	411.56	J/mol×K	657.73	Joback Method
cpg	423.91	J/mol×K	693.36	Joback Method
cpg	435.43	J/mol×K	728.99	Joback Method
cpg	446.18	J/mol×K	764.61	Joback Method
cpg	456.18	J/mol×K	800.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308475&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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