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

Inchi: InChI=1S/C11H13Cl2NO/c1-3-14(11(15)10(12)13)9-6-4-5-8(2)7-9/h4-7,10H,3H2,1-2H3

InchiKey: SAURIVDRNUMSSC-UHFFFAOYSA-N

Formula: C11H13Cl2NO

SMILES: CCN(C(=O)C(Cl)Cl)c1cccc(C)c1

Mol. weight [g/mol]: 246.13

Physical Properties

Property code	Value	Unit	Source
gf	100.08	kJ/mol	Joback Method
hf	-127.12	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	60.19	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.152		Crippen Method
mcvol	178.120	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1658.00		NIST Webbook
tb	623.47	K	Joback Method
tc	845.44	K	Joback Method
tf	379.91	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.87	J/mol×K	623.47	Joback Method
cpg	424.29	J/mol×K	660.46	Joback Method
cpg	436.75	J/mol×K	697.46	Joback Method
cpg	448.31	J/mol×K	734.45	Joback Method
cpg	459.02	J/mol×K	771.45	Joback Method
cpg	468.93	J/mol×K	808.44	Joback Method
cpg	478.09	J/mol×K	845.44	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=U308633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume