Acetamide, 2,2,2-trichloro-N-(3-methylphenyl)-

Other names: Acetamide, N-(3-methylphenyl)-2,2,2-trichloro-
Inchi: InChI=1S/C9H8Cl3NO/c1-6-3-2-4-7(5-6)13-8(14)9(10,11)12/h2-5H,1H3,(H,13,14)
InchiKey: WJTMDWHORSRZQN-UHFFFAOYSA-N
Formula: C9H8Cl3NO
SMILES: Cc1cccc(NC(=O)C(Cl)(Cl)Cl)c1
Mol. weight [g/mol]: 252.53
CAS: 2563-96-4

Physical Properties

Property code	Value	Unit	Source
gf	55.20	kJ/mol	Joback Method
hf	-119.11	kJ/mol	Joback Method
hfus	24.59	kJ/mol	Joback Method
hvap	63.61	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.304		Crippen Method
mcvol	162.180	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1699.00		NIST Webbook
rinpol	1699.00		NIST Webbook
tb	650.08	K	Joback Method
tc	895.40	K	Joback Method
tf	424.90	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.43	J/mol×K	650.08	Joback Method
cpg	361.71	J/mol×K	690.97	Joback Method
cpg	371.03	J/mol×K	731.85	Joback Method
cpg	379.48	J/mol×K	772.74	Joback Method
cpg	387.14	J/mol×K	813.62	Joback Method
cpg	394.09	J/mol×K	854.51	Joback Method

cpg	400.41	J/mol×K	895.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2563964&Units=SI

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

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