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

Inchi: InChI=1S/C11H12Cl3NO/c1-3-15(10(16)11(12,13)14)9-6-4-5-8(2)7-9/h4-7H,3H2,1-2H3

InchiKey: DEQXVMATOARFGZ-UHFFFAOYSA-N

Formula: C11H12Cl3NO

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

Mol. weight [g/mol]: 280.58

Physical Properties

Property code	Value	Unit	Source
gf	93.43	kJ/mol	Joback Method
hf	-146.33	kJ/mol	Joback Method
hfus	27.70	kJ/mol	Joback Method
hvap	63.67	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.718		Crippen Method
mcvol	190.360	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1751.00		NIST Webbook
rinpol	1751.00		NIST Webbook
tb	658.11	K	Joback Method
tc	891.87	K	Joback Method
tf	427.25	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.29	J/mol×K	658.11	Joback Method
cpg	450.77	J/mol×K	697.07	Joback Method
cpg	462.20	J/mol×K	736.03	Joback Method
cpg	472.66	J/mol×K	774.99	Joback Method
cpg	482.25	J/mol×K	813.95	Joback Method
cpg	491.03	J/mol×K	852.91	Joback Method
cpg	499.12	J/mol×K	891.87	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=U308486&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