2,2,2-Trichloro-n-(3,4-dichlorophenyl)acetamide

Inchi: InChI=1S/C8H4Cl5NO/c9-5-2-1-4(3-6(5)10)14-7(15)8(11,12)13/h1-3H,(H,14,15)
InchiKey: HOLWKHGHTNFTIB-UHFFFAOYSA-N
Formula: C8H4Cl5NO
SMILES: O=C(Nc1ccc(Cl)c(Cl)c1)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 307.39
CAS: 22303-30-6

Physical Properties

Property code	Value	Unit	Source
gf	13.29	kJ/mol	Joback Method
hf	-141.42	kJ/mol	Joback Method
hfus	30.01	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.302		Crippen Method
mcvol	172.570	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
tb	707.04	K	Joback Method
tc	963.68	K	Joback Method
tf	485.99	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.50	J/mol×K	707.04	Joback Method
cpg	347.58	J/mol×K	749.81	Joback Method
cpg	353.89	J/mol×K	792.59	Joback Method
cpg	359.50	J/mol×K	835.36	Joback Method
cpg	364.51	J/mol×K	878.13	Joback Method
cpg	368.99	J/mol×K	920.90	Joback Method
cpg	373.03	J/mol×K	963.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22303306&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume