2,2,3-Trichloro-n-phenylpropanamide

Inchi: InChI=1S/C9H8Cl3NO/c10-6-9(11,12)8(14)13-7-4-2-1-3-5-7/h1-5H,6H2,(H,13,14)
InchiKey: HBRQIHMUJNDTOR-UHFFFAOYSA-N
Formula: C9H8Cl3NO
SMILES: O=C(Nc1ccccc1)C(Cl)(Cl)CCl
Mol. weight [g/mol]: 252.53
CAS: 16189-06-3

Physical Properties

Property code	Value	Unit	Source
gf	64.83	kJ/mol	Joback Method
hf	-107.64	kJ/mol	Joback Method
hfus	24.98	kJ/mol	Joback Method
hvap	62.94	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	3.038		Crippen Method
mcvol	162.180	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	645.10	K	Joback Method
tc	889.50	K	Joback Method
tf	412.38	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.97	J/mol×K	645.10	Joback Method
cpg	363.46	J/mol×K	685.83	Joback Method
cpg	372.95	J/mol×K	726.57	Joback Method
cpg	381.52	J/mol×K	767.30	Joback Method
cpg	389.26	J/mol×K	808.03	Joback Method
cpg	396.27	J/mol×K	848.77	Joback Method
cpg	402.62	J/mol×K	889.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16189063&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