Acetamide, N-(2-iodo-4-methylphenyl)-2,2,2-trichloro-

Inchi: InChI=1S/C9H7Cl3INO/c1-5-2-3-7(6(13)4-5)14-8(15)9(10,11)12/h2-4H,1H3,(H,14,15)
InchiKey: IPGQTYZUQGYBNC-UHFFFAOYSA-N
Formula: C9H7Cl3INO
SMILES: Cc1ccc(NC(=O)C(Cl)(Cl)Cl)c(I)c1
Mol. weight [g/mol]: 378.42

Physical Properties

Property code	Value	Unit	Source
gf	103.69	kJ/mol	Joback Method
hf	-53.71	kJ/mol	Joback Method
hfus	28.61	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.908		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	2096.00		NIST Webbook
rinpol	2096.00		NIST Webbook
tb	748.20	K	Joback Method
tc	1019.86	K	Joback Method
tf	495.48	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.40	J/mol×K	748.20	Joback Method
cpg	391.63	J/mol×K	793.48	Joback Method
cpg	399.03	J/mol×K	838.75	Joback Method
cpg	405.72	J/mol×K	884.03	Joback Method
cpg	411.80	J/mol×K	929.31	Joback Method
cpg	417.42	J/mol×K	974.58	Joback Method
cpg	422.67	J/mol×K	1019.86	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=U307221&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