2,2,3-Trichloro-n-(4-chloro-2-nitrophenyl)propana

Inchi: InChI=1S/C9H6Cl4N2O3/c10-4-9(12,13)8(16)14-6-2-1-5(11)3-7(6)15(17)18/h1-3H,4H2,(
InchiKey: UNKOKYAXAPLGTA-UHFFFAOYSA-N
Formula: C9H6Cl4N2O3
SMILES: O=C(Nc1ccc(Cl)cc1[N+](=O)[O-])C(Cl)(Cl)CCl
Mol. weight [g/mol]: 331.97
CAS: 116402-47-2

Physical Properties

Property code	Value	Unit	Source
gf	69.19	kJ/mol	Joback Method
hf	-157.08	kJ/mol	Joback Method
hfus	39.76	kJ/mol	Joback Method
hvap	85.24	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.599		Crippen Method
mcvol	191.840	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
tb	844.33	K	Joback Method
tc	1109.48	K	Joback Method
tf	610.95	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.18	J/mol×K	844.33	Joback Method
cpg	451.17	J/mol×K	888.52	Joback Method
cpg	457.41	J/mol×K	932.71	Joback Method
cpg	463.02	J/mol×K	976.90	Joback Method
cpg	468.09	J/mol×K	1021.10	Joback Method
cpg	472.74	J/mol×K	1065.29	Joback Method
cpg	477.06	J/mol×K	1109.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402472&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

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