N-butyl-2,2,3-trichloro-n-(2-chlorophenyl)propana

Inchi: InChI=1S/C13H15Cl4NO/c1-2-3-8-18(12(19)13(16,17)9-14)11-7-5-4-6-10(11)15/h4-7H,2
InchiKey: XFQQOGAYSCNLAV-UHFFFAOYSA-N
Formula: C13H15Cl4NO
SMILES: CCCCN(C(=O)C(Cl)(Cl)CCl)c1ccccc1Cl
Mol. weight [g/mol]: 343.08
CAS: 116402-43-8

Physical Properties

Property code	Value	Unit	Source
gf	98.34	kJ/mol	Joback Method
hf	-203.35	kJ/mol	Joback Method
hfus	37.07	kJ/mol	Joback Method
hvap	72.50	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.886		Crippen Method
mcvol	230.780	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
tb	741.30	K	Joback Method
tc	969.13	K	Joback Method
tf	479.71	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.98	J/mol×K	741.30	Joback Method
cpg	575.24	J/mol×K	779.27	Joback Method
cpg	586.52	J/mol×K	817.24	Joback Method
cpg	596.91	J/mol×K	855.21	Joback Method
cpg	606.51	J/mol×K	893.19	Joback Method
cpg	615.41	J/mol×K	931.16	Joback Method
cpg	623.69	J/mol×K	969.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402438&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