2,2-Dichloro-n-(4-chlorophenyl)-n-methylpropana

Inchi: InChI=1S/C10H10Cl3NO/c1-10(12,13)9(15)14(2)8-5-3-7(11)4-6-8/h3-6H,1-2H3
InchiKey: ZHUVKKFFFZYYKY-UHFFFAOYSA-N
Formula: C10H10Cl3NO
SMILES: CN(C(=O)C(C)(Cl)Cl)c1ccc(Cl)cc1
Mol. weight [g/mol]: 266.55
CAS: 116558-00-0

Physical Properties

Property code	Value	Unit	Source
gf	85.01	kJ/mol	Joback Method
hf	-125.69	kJ/mol	Joback Method
hfus	25.11	kJ/mol	Joback Method
hvap	61.44	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.497		Crippen Method
mcvol	176.270	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
tb	635.23	K	Joback Method
tc	873.86	K	Joback Method
tf	415.98	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.89	J/mol×K	635.23	Joback Method
cpg	401.75	J/mol×K	675.00	Joback Method
cpg	412.55	J/mol×K	714.77	Joback Method
cpg	422.38	J/mol×K	754.54	Joback Method
cpg	431.33	J/mol×K	794.32	Joback Method
cpg	439.49	J/mol×K	834.09	Joback Method
cpg	446.96	J/mol×K	873.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116558000&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