Cyclopropanecarbamic acid, n-(o-chlorobenzyl)-, ethyl ester

Inchi: InChI=1S/C13H16ClNO2/c1-2-17-13(16)15(11-7-8-11)9-10-5-3-4-6-12(10)14/h3-6,11H,2

InchiKey: GBBRDBFOWFLEKX-UHFFFAOYSA-N

Formula: C13H16ClNO2

SMILES: CCOC(=O)N(Cc1ccccc1Cl)C1CC1

Mol. weight [g/mol]: 253.72

CAS: 116373-53-6

Physical Properties

Property code	Value	Unit	Source
gf	87.04	kJ/mol	Joback Method
hf	-206.80	kJ/mol	Joback Method
hfus	31.22	kJ/mol	Joback Method
hvap	62.97	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.461		Crippen Method
mcvol	189.070	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	661.40	K	Joback Method
tc	879.66	K	Joback Method
tf	427.70	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.36	J/mol×K	661.40	Joback Method
cpg	509.64	J/mol×K	697.78	Joback Method
cpg	523.87	J/mol×K	734.15	Joback Method
cpg	537.11	J/mol×K	770.53	Joback Method
cpg	549.42	J/mol×K	806.91	Joback Method
cpg	560.88	J/mol×K	843.28	Joback Method
cpg	571.54	J/mol×K	879.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116373536&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