Carbanilic acid, m-chloro-, cyclohexyl ester

Inchi: InChI=1S/C13H16ClNO2/c14-10-5-4-6-11(9-10)15-13(16)17-12-7-2-1-3-8-12/h4-6,9,12H
InchiKey: ILBAXXVDXITICM-UHFFFAOYSA-N
Formula: C13H16ClNO2
SMILES: O=C(Nc1cccc(Cl)c1)OC1CCCCC1
Mol. weight [g/mol]: 253.72
CAS: 116373-55-8

Physical Properties

Property code	Value	Unit	Source
gf	29.35	kJ/mol	Joback Method
hf	-239.34	kJ/mol	Joback Method
hfus	27.00	kJ/mol	Joback Method
hvap	67.88	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.221		Crippen Method
mcvol	189.070	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
tb	711.94	K	Joback Method
tc	952.99	K	Joback Method
tf	437.33	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.86	J/mol×K	711.94	Joback Method
cpg	532.43	J/mol×K	752.12	Joback Method
cpg	547.64	J/mol×K	792.29	Joback Method
cpg	561.53	J/mol×K	832.47	Joback Method
cpg	574.14	J/mol×K	872.64	Joback Method
cpg	585.53	J/mol×K	912.82	Joback Method
cpg	595.72	J/mol×K	952.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116373558&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