Carbanilic acid, n-tert-butyl-, beta-chloroethyl ester

Inchi: InChI=1S/C13H18ClNO2/c1-13(2,3)15(12(16)17-10-9-14)11-7-5-4-6-8-11/h4-8H,9-10H2,

InchiKey: CZTLGPZNCWOMBQ-UHFFFAOYSA-N

Formula: C13H18ClNO2

SMILES: CC(C)(C)N(C(=O)OCCCl)c1ccccc1

Mol. weight [g/mol]: 255.74

Physical Properties

Property code	Value	Unit	Source
gf	38.76	kJ/mol	Joback Method
hf	-276.88	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	61.10	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.667		Crippen Method
mcvol	199.930	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
tb	646.45	K	Joback Method
tc	861.77	K	Joback Method
tf	399.66	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.03	J/mol×K	646.45	Joback Method
cpg	528.79	J/mol×K	682.34	Joback Method
cpg	543.43	J/mol×K	718.22	Joback Method
cpg	557.02	J/mol×K	754.11	Joback Method
cpg	569.62	J/mol×K	790.00	Joback Method
cpg	581.29	J/mol×K	825.89	Joback Method
cpg	592.10	J/mol×K	861.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009304&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