Carbanilic acid, 2,4-di-tert-butyl-, 2-chloroethyl ester

Inchi: InChI=1S/C17H26ClNO2/c1-16(2,3)12-7-8-14(13(11-12)17(4,5)6)19-15(20)21-10-9-18/h7

InchiKey: CQYMGMUEIGWFKS-UHFFFAOYSA-N

Formula: C17H26ClNO2

SMILES: CC(C)(C)c1ccc(NC(=O)OCCCl)c(C(C)(C)C)c1

Mol. weight [g/mol]: 311.85

Physical Properties

Property code	Value	Unit	Source
gf	34.63	kJ/mol	Joback Method
hf	-405.19	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	74.42	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	5.069		Crippen Method
mcvol	256.290	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
tb	782.43	K	Joback Method
tc	999.52	K	Joback Method
tf	492.39	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.76	J/mol×K	782.43	Joback Method
cpg	761.88	J/mol×K	818.61	Joback Method
cpg	776.89	J/mol×K	854.79	Joback Method
cpg	790.85	J/mol×K	890.98	Joback Method
cpg	803.84	J/mol×K	927.16	Joback Method
cpg	815.95	J/mol×K	963.34	Joback Method
cpg	827.24	J/mol×K	999.52	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009309&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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