Ethyl N-(3-chloro-4-methylphenyl)carbamate

Other names: Ethyl 3-chloro-4-methylcarbanilate
Inchi: InChI=1S/C10H12ClNO2/c1-3-14-10(13)12-8-5-4-7(2)9(11)6-8/h4-6H,3H2,1-2H3,(H,12,1
InchiKey: KJEXITNRKHKKBH-UHFFFAOYSA-N
Formula: C10H12ClNO2
SMILES: CCOC(=O)Nc1ccc(C)c(Cl)c1
Mol. weight [g/mol]: 213.66
CAS: 85419-40-5

Physical Properties

Property code	Value	Unit	Source
gf	-29.99	kJ/mol	Joback Method
hf	-243.21	kJ/mol	Joback Method
hfus	27.00	kJ/mol	Joback Method
hvap	61.43	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.217		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
tb	628.73	K	Joback Method
tc	847.09	K	Joback Method
tf	408.66	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.92	J/mol×K	628.73	Joback Method
cpg	384.13	J/mol×K	665.12	Joback Method
cpg	395.60	J/mol×K	701.52	Joback Method
cpg	406.35	J/mol×K	737.91	Joback Method
cpg	416.38	J/mol×K	774.30	Joback Method
cpg	425.71	J/mol×K	810.70	Joback Method
cpg	434.34	J/mol×K	847.09	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C85419405&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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