2-(Ethyl(m-tolyl)amino)ethyl 3-chlorobenzoate

Inchi: InChI=1S/C18H20ClNO2/c1-3-20(17-9-4-6-14(2)12-17)10-11-22-18(21)15-7-5-8-16(19)1
InchiKey: UXJBINYPONRUNV-UHFFFAOYSA-N
Formula: C18H20ClNO2
SMILES: CCN(CCOC(=O)c1cccc(Cl)c1)c1cccc(C)c1
Mol. weight [g/mol]: 317.81

Physical Properties

Property code	Value	Unit	Source
gf	171.17	kJ/mol	Joback Method
hf	-157.74	kJ/mol	Joback Method
hfus	39.68	kJ/mol	Joback Method
hvap	77.12	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.332		Crippen Method
mcvol	246.620	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	2453.00		NIST Webbook
tb	800.72	K	Joback Method
tc	1026.94	K	Joback Method
tf	505.05	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.83	J/mol×K	800.72	Joback Method
cpg	706.88	J/mol×K	838.42	Joback Method
cpg	720.73	J/mol×K	876.13	Joback Method
cpg	733.46	J/mol×K	913.83	Joback Method
cpg	745.13	J/mol×K	951.54	Joback Method
cpg	755.79	J/mol×K	989.24	Joback Method
cpg	765.50	J/mol×K	1026.94	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373547&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume