Isophthalic acid, monoamide, N-(2-chlorophenyl)-, ethyl ester

Inchi: InChI=1S/C16H14ClNO3/c1-2-21-16(20)12-7-5-6-11(10-12)15(19)18-14-9-4-3-8-13(14)1

InchiKey: PYVFDIOKDDCZQI-UHFFFAOYSA-N

Formula: C16H14ClNO3

SMILES: CCOC(=O)c1cccc(C(=O)Nc2ccccc2Cl)c1

Mol. weight [g/mol]: 303.74

Physical Properties

Property code	Value	Unit	Source
gf	4.02	kJ/mol	Joback Method
hf	-243.10	kJ/mol	Joback Method
hfus	38.18	kJ/mol	Joback Method
hvap	83.81	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.769		Crippen Method
mcvol	220.010	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	846.56	K	Joback Method
tc	1086.44	K	Joback Method
tf	552.63	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.67	J/mol×K	846.56	Joback Method
cpg	616.33	J/mol×K	886.54	Joback Method
cpg	626.84	J/mol×K	926.52	Joback Method
cpg	636.26	J/mol×K	966.50	Joback Method
cpg	644.64	J/mol×K	1006.48	Joback Method
cpg	652.02	J/mol×K	1046.46	Joback Method
cpg	658.44	J/mol×K	1086.44	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=U345814&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