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

Inchi: InChI=1S/C18H18ClNO3/c1-2-3-11-23-18(22)14-8-6-7-13(12-14)17(21)20-16-10-5-4-9-1

InchiKey: NLAYHBMZFZLFHK-UHFFFAOYSA-N

Formula: C18H18ClNO3

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

Mol. weight [g/mol]: 331.79

Physical Properties

Property code	Value	Unit	Source
gf	20.86	kJ/mol	Joback Method
hf	-284.38	kJ/mol	Joback Method
hfus	43.36	kJ/mol	Joback Method
hvap	88.26	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.549		Crippen Method
mcvol	248.190	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook
tb	892.32	K	Joback Method
tc	1126.04	K	Joback Method
tf	575.17	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.92	J/mol×K	892.32	Joback Method
cpg	728.01	J/mol×K	931.27	Joback Method
cpg	738.93	J/mol×K	970.23	Joback Method
cpg	748.75	J/mol×K	1009.18	Joback Method
cpg	757.51	J/mol×K	1048.13	Joback Method
cpg	765.27	J/mol×K	1087.09	Joback Method
cpg	772.08	J/mol×K	1126.04	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=U345817&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume