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

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

InchiKey: OWPLWPNWUAQDPP-UHFFFAOYSA-N

Formula: C18H18ClNO3

SMILES: CC(C)COC(=O)c1cccc(C(=O)Nc2ccccc2Cl)c1

Mol. weight [g/mol]: 331.79

Physical Properties

Property code	Value	Unit	Source
gf	18.42	kJ/mol	Joback Method
hf	-289.66	kJ/mol	Joback Method
hfus	39.84	kJ/mol	Joback Method
hvap	87.87	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.405		Crippen Method
mcvol	248.190	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	2773.00		NIST Webbook
rinpol	2773.00		NIST Webbook
tb	891.88	K	Joback Method
tc	1128.81	K	Joback Method
tf	560.17	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.48	J/mol×K	891.88	Joback Method
cpg	728.69	J/mol×K	931.37	Joback Method
cpg	739.69	J/mol×K	970.86	Joback Method
cpg	749.54	J/mol×K	1010.34	Joback Method
cpg	758.30	J/mol×K	1049.83	Joback Method
cpg	766.01	J/mol×K	1089.32	Joback Method
cpg	772.73	J/mol×K	1128.81	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=U345816&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume