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

Inchi: InChI=1S/C20H22ClNO3/c1-2-3-4-7-13-25-20(24)16-10-8-9-15(14-16)19(23)22-18-12-6-

InchiKey: CTRWIWVPKFVJRK-UHFFFAOYSA-N

Formula: C20H22ClNO3

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

Mol. weight [g/mol]: 359.85

Physical Properties

Property code	Value	Unit	Source
gf	37.70	kJ/mol	Joback Method
hf	-325.66	kJ/mol	Joback Method
hfus	48.54	kJ/mol	Joback Method
hvap	92.71	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.329		Crippen Method
mcvol	276.370	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
rinpol	3057.00		NIST Webbook
rinpol	3057.00		NIST Webbook
tb	938.08	K	Joback Method
tc	1168.49	K	Joback Method
tf	597.71	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.32	J/mol×K	938.08	Joback Method
cpg	842.71	J/mol×K	976.48	Joback Method
cpg	853.92	J/mol×K	1014.88	Joback Method
cpg	864.01	J/mol×K	1053.29	Joback Method
cpg	873.02	J/mol×K	1091.69	Joback Method
cpg	881.04	J/mol×K	1130.09	Joback Method
cpg	888.10	J/mol×K	1168.49	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=U345820&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