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

Inchi: InChI=1S/C20H22ClNO3/c1-14(2)7-6-12-25-20(24)16-9-5-8-15(13-16)19(23)22-18-11-4-

InchiKey: UYNUQGFBXGCGIM-UHFFFAOYSA-N

Formula: C20H22ClNO3

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

Mol. weight [g/mol]: 359.85

Physical Properties

Property code	Value	Unit	Source
gf	35.26	kJ/mol	Joback Method
hf	-330.94	kJ/mol	Joback Method
hfus	45.02	kJ/mol	Joback Method
hvap	92.33	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.185		Crippen Method
mcvol	276.370	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	3009.00		NIST Webbook
rinpol	3009.00		NIST Webbook
tb	937.64	K	Joback Method
tc	1170.54	K	Joback Method
tf	582.71	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.82	J/mol×K	937.64	Joback Method
cpg	843.29	J/mol×K	976.46	Joback Method
cpg	854.54	J/mol×K	1015.27	Joback Method
cpg	864.62	J/mol×K	1054.09	Joback Method
cpg	873.61	J/mol×K	1092.91	Joback Method
cpg	881.55	J/mol×K	1131.72	Joback Method
cpg	888.51	J/mol×K	1170.54	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=U345819&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