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

Inchi: InChI=1S/C17H16ClNO3/c1-2-10-22-17(21)13-7-5-6-12(11-13)16(20)19-15-9-4-3-8-14(1

InchiKey: JPUUSDPKYMEQIU-UHFFFAOYSA-N

Formula: C17H16ClNO3

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

Mol. weight [g/mol]: 317.77

Physical Properties

Property code	Value	Unit	Source
gf	12.44	kJ/mol	Joback Method
hf	-263.74	kJ/mol	Joback Method
hfus	40.77	kJ/mol	Joback Method
hvap	86.03	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.159		Crippen Method
mcvol	234.100	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook
tb	869.44	K	Joback Method
tc	1105.90	K	Joback Method
tf	563.90	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.87	J/mol×K	869.44	Joback Method
cpg	671.77	J/mol×K	908.85	Joback Method
cpg	682.51	J/mol×K	948.26	Joback Method
cpg	692.15	J/mol×K	987.67	Joback Method
cpg	700.73	J/mol×K	1027.08	Joback Method
cpg	708.32	J/mol×K	1066.49	Joback Method
cpg	714.96	J/mol×K	1105.90	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=U345815&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