Isophthalic acid, isohexyl 4-nitrophenyl ester

Inchi: InChI=1S/C20H21NO6/c1-14(2)5-4-12-26-19(22)15-6-3-7-16(13-15)20(23)27-18-10-8-17
InchiKey: DKGJQQLSRPZOOO-UHFFFAOYSA-N
Formula: C20H21NO6
SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)Oc2ccc([N+](=O)[O-])cc2)c1
Mol. weight [g/mol]: 371.38

Physical Properties

Property code	Value	Unit	Source
gf	-111.65	kJ/mol	Joback Method
hf	-511.65	kJ/mol	Joback Method
hfus	48.27	kJ/mol	Joback Method
hvap	100.51	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	4.407		Crippen Method
mcvol	277.440	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	3133.00		NIST Webbook
rinpol	3133.00		NIST Webbook
tb	1024.30	K	Joback Method
tc	1271.22	K	Joback Method
tf	665.97	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.34	J/mol×K	1024.30	Joback Method
cpg	886.19	J/mol×K	1065.45	Joback Method
cpg	894.56	J/mol×K	1106.61	Joback Method
cpg	901.53	J/mol×K	1147.76	Joback Method
cpg	907.13	J/mol×K	1188.91	Joback Method
cpg	911.41	J/mol×K	1230.07	Joback Method
cpg	914.43	J/mol×K	1271.22	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=U344682&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