Isophthalic acid, 4-cyanophenyl isobutyl ester

Inchi: InChI=1S/C19H17NO4/c1-13(2)12-23-18(21)15-4-3-5-16(10-15)19(22)24-17-8-6-14(11-2
InchiKey: XCGVXXUUHUSSIB-UHFFFAOYSA-N
Formula: C19H17NO4
SMILES: CC(C)COC(=O)c1cccc(C(=O)Oc2ccc(C#N)cc2)c1
Mol. weight [g/mol]: 323.34

Physical Properties

Property code	Value	Unit	Source
gf	-22.44	kJ/mol	Joback Method
hf	-315.37	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	92.17	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	3.590		Crippen Method
mcvol	247.310	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	2765.00		NIST Webbook
tb	951.66	K	Joback Method
tc	1192.50	K	Joback Method
tf	576.08	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.24	J/mol×K	951.66	Joback Method
cpg	746.54	J/mol×K	991.80	Joback Method
cpg	755.52	J/mol×K	1031.94	Joback Method
cpg	763.22	J/mol×K	1072.08	Joback Method
cpg	769.67	J/mol×K	1112.22	Joback Method
cpg	774.90	J/mol×K	1152.36	Joback Method
cpg	778.94	J/mol×K	1192.50	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=U344488&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