Isophthalic acid, 4-cyanophenyl pentyl ester

Inchi: InChI=1S/C20H19NO4/c1-2-3-4-12-24-19(22)16-6-5-7-17(13-16)20(23)25-18-10-8-15(14
InchiKey: NLOHWJYPAGLFHN-UHFFFAOYSA-N
Formula: C20H19NO4
SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C#N)cc2)c1
Mol. weight [g/mol]: 337.37

Physical Properties

Property code	Value	Unit	Source
gf	-11.58	kJ/mol	Joback Method
hf	-330.73	kJ/mol	Joback Method
hfus	41.94	kJ/mol	Joback Method
hvap	94.78	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.124		Crippen Method
mcvol	261.400	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2930.00		NIST Webbook
rinpol	2930.00		NIST Webbook
tb	974.98	K	Joback Method
tc	1211.86	K	Joback Method
tf	602.35	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.83	J/mol×K	974.98	Joback Method
cpg	803.17	J/mol×K	1014.46	Joback Method
cpg	812.20	J/mol×K	1053.94	Joback Method
cpg	819.98	J/mol×K	1093.42	Joback Method
cpg	826.52	J/mol×K	1132.90	Joback Method
cpg	831.88	J/mol×K	1172.38	Joback Method
cpg	836.07	J/mol×K	1211.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U344490&Units=SI

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