Isophthalic acid, 4-cyanophenyl propyl ester

Inchi: InChI=1S/C18H15NO4/c1-2-10-22-17(20)14-4-3-5-15(11-14)18(21)23-16-8-6-13(12-19)7
InchiKey: BGYBSNFHMHLZED-UHFFFAOYSA-N
Formula: C18H15NO4
SMILES: CCCOC(=O)c1cccc(C(=O)Oc2ccc(C#N)cc2)c1
Mol. weight [g/mol]: 309.32

Physical Properties

Property code	Value	Unit	Source
gf	-28.42	kJ/mol	Joback Method
hf	-289.45	kJ/mol	Joback Method
hfus	36.76	kJ/mol	Joback Method
hvap	90.33	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.344		Crippen Method
mcvol	233.220	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook
tb	929.22	K	Joback Method
tc	1169.24	K	Joback Method
tf	579.81	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.30	J/mol×K	929.22	Joback Method
cpg	689.42	J/mol×K	969.22	Joback Method
cpg	698.29	J/mol×K	1009.23	Joback Method
cpg	705.94	J/mol×K	1049.23	Joback Method
cpg	712.40	J/mol×K	1089.23	Joback Method
cpg	717.70	J/mol×K	1129.23	Joback Method
cpg	721.85	J/mol×K	1169.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344487&Units=SI
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

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