Isophthalic acid, 4-cyanophenyl ethyl ester

Inchi: InChI=1S/C17H13NO4/c1-2-21-16(19)13-4-3-5-14(10-13)17(20)22-15-8-6-12(11-18)7-9-
InchiKey: IVJZHNAPZGRRQB-UHFFFAOYSA-N
Formula: C17H13NO4
SMILES: CCOC(=O)c1cccc(C(=O)Oc2ccc(C#N)cc2)c1
Mol. weight [g/mol]: 295.29

Physical Properties

Property code	Value	Unit	Source
gf	-36.84	kJ/mol	Joback Method
hf	-268.81	kJ/mol	Joback Method
hfus	34.17	kJ/mol	Joback Method
hvap	88.10	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	2.954		Crippen Method
mcvol	219.130	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	2606.00		NIST Webbook
rinpol	2606.00		NIST Webbook
tb	906.34	K	Joback Method
tc	1149.08	K	Joback Method
tf	568.54	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.58	J/mol×K	906.34	Joback Method
cpg	633.53	J/mol×K	946.80	Joback Method
cpg	642.26	J/mol×K	987.25	Joback Method
cpg	649.79	J/mol×K	1027.71	Joback Method
cpg	656.15	J/mol×K	1068.17	Joback Method
cpg	661.35	J/mol×K	1108.63	Joback Method
cpg	665.42	J/mol×K	1149.08	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=U344486&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

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