Isophthalic acid, 4-cyanophenyl heptyl ester

Inchi: InChI=1S/C22H23NO4/c1-2-3-4-5-6-14-26-21(24)18-8-7-9-19(15-18)22(25)27-20-12-10-1
InchiKey: CEFBIYYQBAUEHP-UHFFFAOYSA-N
Formula: C22H23NO4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C#N)cc2)c1
Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
gf	5.26	kJ/mol	Joback Method
hf	-372.01	kJ/mol	Joback Method
hfus	47.12	kJ/mol	Joback Method
hvap	99.23	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	4.905		Crippen Method
mcvol	289.580	ml/mol	McGowan Method
pc	1444.64	kPa	Joback Method
rinpol	3157.00		NIST Webbook
rinpol	3157.00		NIST Webbook
tb	1020.74	K	Joback Method
tc	1257.88	K	Joback Method
tf	624.89	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.76	J/mol×K	1020.74	Joback Method
cpg	919.22	J/mol×K	1060.26	Joback Method
cpg	928.32	J/mol×K	1099.79	Joback Method
cpg	936.09	J/mol×K	1139.31	Joback Method
cpg	942.60	J/mol×K	1178.83	Joback Method
cpg	947.87	J/mol×K	1218.36	Joback Method
cpg	951.95	J/mol×K	1257.88	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=U344493&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