Isophthalic acid, 4-cyanophenyl isohexyl ester

Inchi: InChI=1S/C21H21NO4/c1-15(2)5-4-12-25-20(23)17-6-3-7-18(13-17)21(24)26-19-10-8-16
InchiKey: WCRATETXNJRCPF-UHFFFAOYSA-N
Formula: C21H21NO4
SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)Oc2ccc(C#N)cc2)c1
Mol. weight [g/mol]: 351.40

Physical Properties

Property code	Value	Unit	Source
gf	-5.60	kJ/mol	Joback Method
hf	-356.65	kJ/mol	Joback Method
hfus	41.01	kJ/mol	Joback Method
hvap	96.62	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.370		Crippen Method
mcvol	275.490	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	2995.00		NIST Webbook
rinpol	2995.00		NIST Webbook
tb	997.42	K	Joback Method
tc	1236.01	K	Joback Method
tf	598.62	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.94	J/mol×K	997.42	Joback Method
cpg	861.36	J/mol×K	1037.19	Joback Method
cpg	870.41	J/mol×K	1076.95	Joback Method
cpg	878.14	J/mol×K	1116.72	Joback Method
cpg	884.58	J/mol×K	1156.48	Joback Method
cpg	889.77	J/mol×K	1196.25	Joback Method
cpg	893.76	J/mol×K	1236.01	Joback Method

Sources

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=U344491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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