Isophthalic acid, 4-cyanophenyl decyl ester

Inchi: InChI=1S/C25H29NO4/c1-2-3-4-5-6-7-8-9-17-29-24(27)21-11-10-12-22(18-21)25(28)30-
InchiKey: XAJUEYZKKKYKKW-UHFFFAOYSA-N
Formula: C25H29NO4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C#N)cc2)c1
Mol. weight [g/mol]: 407.50

Physical Properties

Property code	Value	Unit	Source
gf	30.52	kJ/mol	Joback Method
hf	-433.93	kJ/mol	Joback Method
hfus	54.89	kJ/mol	Joback Method
hvap	105.91	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.075		Crippen Method
mcvol	331.850	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	3467.00		NIST Webbook
rinpol	3467.00		NIST Webbook
tb	1089.38	K	Joback Method
tc	1334.14	K	Joback Method
tf	658.70	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1086.28	J/mol×K	1089.38	Joback Method
cpg	1096.87	J/mol×K	1130.17	Joback Method
cpg	1105.95	J/mol×K	1170.97	Joback Method
cpg	1113.58	J/mol×K	1211.76	Joback Method
cpg	1119.83	J/mol×K	1252.55	Joback Method
cpg	1124.75	J/mol×K	1293.35	Joback Method
cpg	1128.42	J/mol×K	1334.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344495&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

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