

Isophthalic acid, 4-cyanophenyl nonyl ester

Inchi:	InChI=1S/C24H27NO4/c1-2-3-4-5-6-7-8-16-28-23(26)20-10-9-11-21(17-20)24(27)29-22-
InchiKey:	PIBVDGFQSUXRRE-UHFFFAOYSA-N
Formula:	C24H27NO4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C#N)cc2)c1
Mol. weight [g/mol]:	393.48

Physical Properties

Property code	Value	Unit	Source
gf	22.10	kJ/mol	Joback Method
hf	-413.29	kJ/mol	Joback Method
hfus	52.30	kJ/mol	Joback Method
hvap	103.68	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	5.685		Crippen Method
mvol	317.760	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	3364.00		NIST Webbook
rinpol	3364.00		NIST Webbook
tb	1066.50	K	Joback Method
tc	1307.68	K	Joback Method
tf	647.43	K	Joback Method
vc	1.238	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.68	J/mol×K	1066.50	Joback Method
cpg	1037.23	J/mol×K	1106.70	Joback Method
cpg	1046.32	J/mol×K	1146.89	Joback Method
cpg	1054.02	J/mol×K	1187.09	Joback Method
cpg	1060.37	J/mol×K	1227.29	Joback Method
cpg	1065.44	J/mol×K	1267.48	Joback Method
cpg	1069.28	J/mol×K	1307.68	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=U344494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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