Succinic acid, di(4-cyanophenyl) ester

Inchi: InChI=1S/C18H12N2O4/c19-11-13-1-5-15(6-2-13)23-17(21)9-10-18(22)24-16-7-3-14(12-
InchiKey: ZSXZIPXJWLPCKL-UHFFFAOYSA-N
Formula: C18H12N2O4
SMILES: N#Cc1ccc(OC(=O)CCC(=O)Oc2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 320.30

Physical Properties

Property code	Value	Unit	Source
gf	104.76	kJ/mol	Joback Method
hf	-124.57	kJ/mol	Joback Method
hfus	38.27	kJ/mol	Joback Method
hvap	100.81	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	2.721		Crippen Method
mcvol	234.600	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	1031.30	K	Joback Method
tc	1282.69	K	Joback Method
tf	644.80	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.46	J/mol×K	1031.30	Joback Method
cpg	684.88	J/mol×K	1073.20	Joback Method
cpg	690.04	J/mol×K	1115.10	Joback Method
cpg	693.98	J/mol×K	1156.99	Joback Method
cpg	696.73	J/mol×K	1198.89	Joback Method
cpg	698.31	J/mol×K	1240.79	Joback Method
cpg	698.75	J/mol×K	1282.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360712&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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