Succinic acid, 4-cyanophenyl 4-isopropylphenyl ester

Inchi: InChI=1S/C20H19NO4/c1-14(2)16-5-9-18(10-6-16)25-20(23)12-11-19(22)24-17-7-3-15(1

InchiKey: CJPYVMGHKQAIIB-UHFFFAOYSA-N

Formula: C20H19NO4

SMILES: CC(C)c1ccc(OC(=O)CCC(=O)Oc2ccc(C#N)cc2)cc1

Mol. weight [g/mol]: 337.37

Physical Properties

Property code	Value	Unit	Source
gf	-14.02	kJ/mol	Joback Method
hf	-336.01	kJ/mol	Joback Method
hfus	38.42	kJ/mol	Joback Method
hvap	94.39	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	3.973		Crippen Method
mcvol	261.400	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	2829.00		NIST Webbook
tb	974.54	K	Joback Method
tc	1213.84	K	Joback Method
tf	587.35	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.30	J/mol×K	974.54	Joback Method
cpg	803.67	J/mol×K	1014.42	Joback Method
cpg	812.70	J/mol×K	1054.31	Joback Method
cpg	820.42	J/mol×K	1094.19	Joback Method
cpg	826.89	J/mol×K	1134.07	Joback Method
cpg	832.11	J/mol×K	1173.95	Joback Method
cpg	836.15	J/mol×K	1213.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360708&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