Succinic acid, 4-cyanophenyl 3,4-dimethylphenyl ester

Inchi: InChI=1S/C19H17NO4/c1-13-3-6-17(11-14(13)2)24-19(22)10-9-18(21)23-16-7-4-15(12-2

InchiKey: YJADWINZDREEFX-UHFFFAOYSA-N

Formula: C19H17NO4

SMILES: Cc1ccc(OC(=O)CCC(=O)Oc2ccc(C#N)cc2)cc1C

Mol. weight [g/mol]: 323.34

Physical Properties

Property code	Value	Unit	Source
gf	-29.63	kJ/mol	Joback Method
hf	-321.56	kJ/mol	Joback Method
hfus	38.96	kJ/mol	Joback Method
hvap	93.22	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.466		Crippen Method
mcvol	247.310	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
tb	957.08	K	Joback Method
tc	1195.87	K	Joback Method
tf	603.60	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.05	J/mol×K	957.08	Joback Method
cpg	744.16	J/mol×K	996.88	Joback Method
cpg	752.98	J/mol×K	1036.68	Joback Method
cpg	760.53	J/mol×K	1076.48	Joback Method
cpg	766.81	J/mol×K	1116.27	Joback Method
cpg	771.87	J/mol×K	1156.07	Joback Method
cpg	775.72	J/mol×K	1195.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360707&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

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