Succinic acid, 4-cyanophenyl N,N-diethyl-2-aminoethyl ester

Inchi: InChI=1S/C17H22N2O4/c1-3-19(4-2)11-12-22-16(20)9-10-17(21)23-15-7-5-14(13-18)6-8

InchiKey: JFIFVHWRTNXPPQ-UHFFFAOYSA-N

Formula: C17H22N2O4

SMILES: CCN(CC)CCOC(=O)CCC(=O)Oc1ccc(C#N)cc1

Mol. weight [g/mol]: 318.37

Physical Properties

Property code	Value	Unit	Source
gf	-28.84	kJ/mol	Joback Method
hf	-426.34	kJ/mol	Joback Method
hfus	43.54	kJ/mol	Joback Method
hvap	87.21	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.129		Crippen Method
mcvol	252.870	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	2474.00		NIST Webbook
tb	887.12	K	Joback Method
tc	1100.49	K	Joback Method
tf	562.07	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.92	J/mol×K	887.12	Joback Method
cpg	781.24	J/mol×K	922.68	Joback Method
cpg	792.48	J/mol×K	958.24	Joback Method
cpg	802.68	J/mol×K	993.80	Joback Method
cpg	811.86	J/mol×K	1029.37	Joback Method
cpg	820.05	J/mol×K	1064.93	Joback Method
cpg	827.26	J/mol×K	1100.49	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360710&Units=SI

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