Succinic acid, 4-cyanophenyl 2-(dimethylamino)ethyl ester

Inchi: InChI=1S/C15H18N2O4/c1-17(2)9-10-20-14(18)7-8-15(19)21-13-5-3-12(11-16)4-6-13/h3

InchiKey: VMINWLJHVACEQJ-UHFFFAOYSA-N

Formula: C15H18N2O4

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

Mol. weight [g/mol]: 290.31

Physical Properties

Property code	Value	Unit	Source
gf	-45.68	kJ/mol	Joback Method
hf	-385.06	kJ/mol	Joback Method
hfus	38.36	kJ/mol	Joback Method
hvap	82.75	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.349		Crippen Method
mcvol	224.690	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	2314.00		NIST Webbook
tb	841.36	K	Joback Method
tc	1055.83	K	Joback Method
tf	539.53	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.24	J/mol×K	841.36	Joback Method
cpg	668.06	J/mol×K	877.11	Joback Method
cpg	678.87	J/mol×K	912.85	Joback Method
cpg	688.71	J/mol×K	948.60	Joback Method
cpg	697.58	J/mol×K	984.34	Joback Method
cpg	705.52	J/mol×K	1020.09	Joback Method
cpg	712.53	J/mol×K	1055.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360711&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