Succinic acid, cyclohexylmethyl 4-cyanophenyl ester

Inchi: InChI=1S/C18H21NO4/c19-12-14-6-8-16(9-7-14)23-18(21)11-10-17(20)22-13-15-4-2-1-3

InchiKey: KNFWMKBPIHMKGG-UHFFFAOYSA-N

Formula: C18H21NO4

SMILES: N#Cc1ccc(OC(=O)CCC(=O)OCC2CCCCC2)cc1

Mol. weight [g/mol]: 315.36

Physical Properties

Property code	Value	Unit	Source
gf	-106.75	kJ/mol	Joback Method
hf	-460.19	kJ/mol	Joback Method
hfus	34.94	kJ/mol	Joback Method
hvap	87.82	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.367		Crippen Method
mcvol	246.120	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2665.00		NIST Webbook
rinpol	2665.00		NIST Webbook
tb	917.11	K	Joback Method
tc	1151.63	K	Joback Method
tf	548.25	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.55	J/mol×K	917.11	Joback Method
cpg	790.37	J/mol×K	956.20	Joback Method
cpg	801.72	J/mol×K	995.28	Joback Method
cpg	811.62	J/mol×K	1034.37	Joback Method
cpg	820.11	J/mol×K	1073.46	Joback Method
cpg	827.20	J/mol×K	1112.54	Joback Method
cpg	832.93	J/mol×K	1151.63	Joback Method

Sources

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=U389814&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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