Succinic acid, 6-chlorohexyl 4-cyanophenyl ester

Inchi: InChI=1S/C17H20ClNO4/c18-11-3-1-2-4-12-22-16(20)9-10-17(21)23-15-7-5-14(13-19)6-

InchiKey: YOKNTAJUAZKDJU-UHFFFAOYSA-N

Formula: C17H20ClNO4

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

Mol. weight [g/mol]: 337.80

Physical Properties

Property code	Value	Unit	Source
gf	-151.55	kJ/mol	Joback Method
hf	-509.61	kJ/mol	Joback Method
hfus	44.71	kJ/mol	Joback Method
hvap	89.55	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.586		Crippen Method
mcvol	255.130	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2743.00		NIST Webbook
rinpol	2743.00		NIST Webbook
tb	912.11	K	Joback Method
tc	1130.58	K	Joback Method
tf	559.52	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.58	J/mol×K	912.11	Joback Method
cpg	760.70	J/mol×K	948.52	Joback Method
cpg	770.75	J/mol×K	984.93	Joback Method
cpg	779.74	J/mol×K	1021.34	Joback Method
cpg	787.70	J/mol×K	1057.75	Joback Method
cpg	794.64	J/mol×K	1094.16	Joback Method
cpg	800.58	J/mol×K	1130.58	Joback Method

Sources

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=U360706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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