Succinic acid, 2-chloroethyl 4-cyanophenyl ester

Inchi: InChI=1S/C13H12ClNO4/c14-7-8-18-12(16)5-6-13(17)19-11-3-1-10(9-15)2-4-11/h1-4H,5

InchiKey: DGPKDEUHHJQHQR-UHFFFAOYSA-N

Formula: C13H12ClNO4

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

Mol. weight [g/mol]: 281.69

Physical Properties

Property code	Value	Unit	Source
gf	-185.23	kJ/mol	Joback Method
hf	-427.05	kJ/mol	Joback Method
hfus	34.35	kJ/mol	Joback Method
hvap	80.64	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.026		Crippen Method
mcvol	198.770	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	2282.00		NIST Webbook
rinpol	2282.00		NIST Webbook
tb	820.59	K	Joback Method
tc	1044.14	K	Joback Method
tf	514.44	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.78	J/mol×K	820.59	Joback Method
cpg	538.70	J/mol×K	857.85	Joback Method
cpg	547.71	J/mol×K	895.11	Joback Method
cpg	555.82	J/mol×K	932.36	Joback Method
cpg	563.02	J/mol×K	969.62	Joback Method
cpg	569.33	J/mol×K	1006.88	Joback Method
cpg	574.76	J/mol×K	1044.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360702&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

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