Succinic acid, 2-chlorophenyl N,N-diethyl-2-aminoethyl ester

Inchi: InChI=1S/C16H22ClNO4/c1-3-18(4-2)11-12-21-15(19)9-10-16(20)22-14-8-6-5-7-13(14)1

InchiKey: MFMXUEGOSSKJTD-UHFFFAOYSA-N

Formula: C16H22ClNO4

SMILES: CCN(CC)CCOC(=O)CCC(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 327.80

Physical Properties

Property code	Value	Unit	Source
gf	-182.37	kJ/mol	Joback Method
hf	-586.32	kJ/mol	Joback Method
hfus	43.64	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.911		Crippen Method
mcvol	249.640	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	2340.00		NIST Webbook
tb	799.59	K	Joback Method
tc	1003.88	K	Joback Method
tf	515.73	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.92	J/mol×K	799.59	Joback Method
cpg	729.99	J/mol×K	833.64	Joback Method
cpg	743.04	J/mol×K	867.69	Joback Method
cpg	755.10	J/mol×K	901.73	Joback Method
cpg	766.19	J/mol×K	935.78	Joback Method
cpg	776.34	J/mol×K	969.83	Joback Method
cpg	785.56	J/mol×K	1003.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357558&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