Succinic acid, 5-fluoro-2-nitrophenyl 2-chloroethyl ester

Inchi: InChI=1S/C12H11ClFNO6/c13-5-6-20-11(16)3-4-12(17)21-10-7-8(14)1-2-9(10)15(18)19/

InchiKey: RXQRLUKPKMZUBT-UHFFFAOYSA-N

Formula: C12H11ClFNO6

SMILES: O=C(CCC(=O)Oc1cc(F)ccc1[N+](=O)[O-])OCCCl

Mol. weight [g/mol]: 319.67

Physical Properties

Property code	Value	Unit	Source
gf	-495.72	kJ/mol	Joback Method
hf	-789.63	kJ/mol	Joback Method
hfus	44.31	kJ/mol	Joback Method
hvap	84.38	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.202		Crippen Method
mcvol	202.490	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	2244.00		NIST Webbook
tb	851.72	K	Joback Method
tc	1078.47	K	Joback Method
tf	594.90	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.23	J/mol×K	851.72	Joback Method
cpg	568.61	J/mol×K	889.51	Joback Method
cpg	577.01	J/mol×K	927.30	Joback Method
cpg	584.44	J/mol×K	965.10	Joback Method
cpg	590.88	J/mol×K	1002.89	Joback Method
cpg	596.36	J/mol×K	1040.68	Joback Method
cpg	600.87	J/mol×K	1078.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357980&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