Succinic acid, ethyl 2-fluoro-5-nitrobenzyl ester

Inchi: InChI=1S/C13H14FNO6/c1-2-20-12(16)5-6-13(17)21-8-9-7-10(15(18)19)3-4-11(9)14/h3-4

InchiKey: VNUDLHCCOSVCDW-UHFFFAOYSA-N

Formula: C13H14FNO6

SMILES: CCOC(=O)CCC(=O)OCc1cc([N+](=O)[O-])ccc1F

Mol. weight [g/mol]: 299.25

Physical Properties

Property code	Value	Unit	Source
gf	-475.37	kJ/mol	Joback Method
hf	-794.53	kJ/mol	Joback Method
hfus	42.70	kJ/mol	Joback Method
hvap	82.22	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.120		Crippen Method
mcvol	204.340	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	837.17	K	Joback Method
tc	1058.48	K	Joback Method
tf	576.25	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.28	J/mol×K	837.17	Joback Method
cpg	604.16	J/mol×K	874.05	Joback Method
cpg	614.04	J/mol×K	910.94	Joback Method
cpg	622.91	J/mol×K	947.82	Joback Method
cpg	630.77	J/mol×K	984.71	Joback Method
cpg	637.65	J/mol×K	1021.59	Joback Method
cpg	643.53	J/mol×K	1058.48	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=U380923&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