Succinic acid, di(2-fluoro-5-nitrobenzyl) ester

Inchi: InChI=1S/C18H14F2N2O8/c19-15-3-1-13(21(25)26)7-11(15)9-29-17(23)5-6-18(24)30-10
InchiKey: QAKCIUIJURYERK-UHFFFAOYSA-N
Formula: C18H14F2N2O8
SMILES: O=C(CCC(=O)OCc1cc([N+](=O)[O-])ccc1F)OCc1cc([N+](=O)[O-])ccc1F
Mol. weight [g/mol]: 424.31

Physical Properties

Property code	Value	Unit	Source
gf	-499.38	kJ/mol	Joback Method
hf	-891.01	kJ/mol	Joback Method
hfus	63.36	kJ/mol	Joback Method
hvap	112.72	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	3.348		Crippen Method
mcvol	270.220	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	3144.00		NIST Webbook
rinpol	3144.00		NIST Webbook
tb	1139.32	K	Joback Method
tc	1399.61	K	Joback Method
tf	828.26	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.08	J/mol×K	1139.32	Joback Method
cpg	848.10	J/mol×K	1182.70	Joback Method
cpg	850.61	J/mol×K	1226.08	Joback Method
cpg	851.63	J/mol×K	1269.46	Joback Method
cpg	851.20	J/mol×K	1312.84	Joback Method
cpg	849.36	J/mol×K	1356.23	Joback Method
cpg	846.15	J/mol×K	1399.61	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=U380934&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