Succinic acid, 2-fluoro-5-nitrobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H24FNO6/c1-4-5-16(12(2)3)26-18(22)9-8-17(21)25-11-13-10-14(20(23)24)

InchiKey: KURQUPZTMZRATD-UHFFFAOYSA-N

Formula: C18H24FNO6

SMILES: CCCC(OC(=O)CCC(=O)OCc1cc([N+](=O)[O-])ccc1F)C(C)C

Mol. weight [g/mol]: 369.38

Physical Properties

Property code	Value	Unit	Source
gf	-438.15	kJ/mol	Joback Method
hf	-908.29	kJ/mol	Joback Method
hfus	48.61	kJ/mol	Joback Method
hvap	92.57	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	3.925		Crippen Method
mcvol	274.790	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
tb	950.69	K	Joback Method
tc	1173.34	K	Joback Method
tf	602.60	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.12	J/mol×K	950.69	Joback Method
cpg	889.12	J/mol×K	987.80	Joback Method
cpg	899.81	J/mol×K	1024.91	Joback Method
cpg	909.23	J/mol×K	1062.01	Joback Method
cpg	917.41	J/mol×K	1099.12	Joback Method
cpg	924.35	J/mol×K	1136.23	Joback Method
cpg	930.09	J/mol×K	1173.34	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=U380927&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