

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

Inchi:	InChI=1S/C22H32FNO6/c1-2-3-4-5-6-7-8-9-10-15-29-21(25)13-14-22(26)30-17-18-16-19
InchiKey:	ZJJUVAVMVHDQOI-UHFFFAOYSA-N
Formula:	C22H32FNO6
SMILES:	CCCCCCCCCOC(=O)CCC(=O)OCc1cc([N+](=O)[O-])ccc1F
Mol. weight [g/mol]:	425.49

Physical Properties

Property code	Value	Unit	Source
gf	-399.59	kJ/mol	Joback Method
hf	-980.29	kJ/mol	Joback Method
hfus	66.01	kJ/mol	Joback Method
hvap	102.25	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.631		Crippen Method
mvol	331.150	ml/mol	McGowan Method
pc	1133.67	kPa	Joback Method
rinpol	3013.00		NIST Webbook
rinpol	3013.00		NIST Webbook
tb	1043.09	K	Joback Method
tc	1277.17	K	Joback Method
tf	677.68	K	Joback Method
vc	1.308	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1113.70	J/molxK	1043.09	Joback Method
cpg	1126.20	J/molxK	1082.10	Joback Method
cpg	1137.17	J/molxK	1121.12	Joback Method
cpg	1146.66	J/molxK	1160.13	Joback Method
cpg	1154.70	J/molxK	1199.14	Joback Method
cpg	1161.34	J/molxK	1238.15	Joback Method
cpg	1166.63	J/molxK	1277.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U380933&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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