Sebacic acid, 3-nitro-4-fluorobenzyl pentyl ester

Inchi: InChI=1S/C22H32FNO6/c1-2-3-10-15-29-21(25)11-8-6-4-5-7-9-12-22(26)30-17-18-13-14

InchiKey: ADYYHHKMRYMZRU-UHFFFAOYSA-N

Formula: C22H32FNO6

SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(F)c([N+](=O)[O-])c1

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
mcvol	331.150	ml/mol	McGowan Method
pc	1133.67	kPa	Joback Method
rinpol	3061.00		NIST Webbook
rinpol	3061.00		NIST Webbook
tb	1043.09	K	Joback Method
tc	1277.17	K	Joback Method
tf	677.68	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380698&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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