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

Inchi: InChI=1S/C21H30FNO6/c1-16(2)14-28-20(24)9-7-5-3-4-6-8-10-21(25)29-15-17-11-12-18

InchiKey: RYVWFJDYXZDBJH-UHFFFAOYSA-N

Formula: C21H30FNO6

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

Mol. weight [g/mol]: 411.46

Physical Properties

Property code	Value	Unit	Source
gf	-410.45	kJ/mol	Joback Method
hf	-964.93	kJ/mol	Joback Method
hfus	59.90	kJ/mol	Joback Method
hvap	99.64	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	5.097		Crippen Method
mcvol	317.060	ml/mol	McGowan Method
pc	1217.44	kPa	Joback Method
rinpol	2935.00		NIST Webbook
rinpol	2935.00		NIST Webbook
tb	1019.77	K	Joback Method
tc	1248.93	K	Joback Method
tf	651.41	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.96	J/mol×K	1019.77	Joback Method
cpg	1066.26	J/mol×K	1057.96	Joback Method
cpg	1077.10	J/mol×K	1096.16	Joback Method
cpg	1086.51	J/mol×K	1134.35	Joback Method
cpg	1094.55	J/mol×K	1172.54	Joback Method
cpg	1101.23	J/mol×K	1210.73	Joback Method
cpg	1106.61	J/mol×K	1248.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380695&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
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