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

Inchi: InChI=1S/C23H34FNO6/c1-2-3-4-11-16-30-22(26)12-9-7-5-6-8-10-13-23(27)31-18-19-14

InchiKey: MPQLCUUHOIGAKZ-UHFFFAOYSA-N

Formula: C23H34FNO6

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

Mol. weight [g/mol]: 439.52

Physical Properties

Property code	Value	Unit	Source
gf	-391.17	kJ/mol	Joback Method
hf	-1000.93	kJ/mol	Joback Method
hfus	68.60	kJ/mol	Joback Method
hvap	104.48	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.021		Crippen Method
mcvol	345.240	ml/mol	McGowan Method
pc	1063.79	kPa	Joback Method
rinpol	3152.00		NIST Webbook
rinpol	3152.00		NIST Webbook
tb	1065.97	K	Joback Method
tc	1306.31	K	Joback Method
tf	688.95	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1174.18	J/mol×K	1065.97	Joback Method
cpg	1186.83	J/mol×K	1106.03	Joback Method
cpg	1197.84	J/mol×K	1146.08	Joback Method
cpg	1207.27	J/mol×K	1186.14	Joback Method
cpg	1215.17	J/mol×K	1226.20	Joback Method
cpg	1221.60	J/mol×K	1266.25	Joback Method
cpg	1226.61	J/mol×K	1306.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380699&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