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

Inchi: InChI=1S/C19H26FNO6/c1-2-26-18(22)9-7-5-3-4-6-8-10-19(23)27-14-15-11-12-16(20)17
InchiKey: OFVOAQRKGNGTTG-UHFFFAOYSA-N
Formula: C19H26FNO6
SMILES: CCOC(=O)CCCCCCCCC(=O)OCc1ccc(F)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 383.41

Physical Properties

Property code	Value	Unit	Source
gf	-424.85	kJ/mol	Joback Method
hf	-918.37	kJ/mol	Joback Method
hfus	58.24	kJ/mol	Joback Method
hvap	95.57	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.461		Crippen Method
mcvol	288.880	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	2789.00		NIST Webbook
rinpol	2789.00		NIST Webbook
tb	974.45	K	Joback Method
tc	1196.30	K	Joback Method
tf	643.87	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.80	J/mol×K	974.45	Joback Method
cpg	946.88	J/mol×K	1011.43	Joback Method
cpg	957.67	J/mol×K	1048.40	Joback Method
cpg	967.19	J/mol×K	1085.38	Joback Method
cpg	975.46	J/mol×K	1122.35	Joback Method
cpg	982.51	J/mol×K	1159.33	Joback Method
cpg	988.38	J/mol×K	1196.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380693&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

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