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

Inchi: InChI=1S/C24H36FNO6/c1-2-3-4-9-12-17-31-23(27)13-10-7-5-6-8-11-14-24(28)32-19-20
InchiKey: WRKXYNGOCDVQKM-UHFFFAOYSA-N
Formula: C24H36FNO6
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(F)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 453.54

Physical Properties

Property code	Value	Unit	Source
gf	-382.75	kJ/mol	Joback Method
hf	-1021.57	kJ/mol	Joback Method
hfus	71.19	kJ/mol	Joback Method
hvap	106.70	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	6.411		Crippen Method
mcvol	359.330	ml/mol	McGowan Method
pc	1000.18	kPa	Joback Method
rinpol	3244.00		NIST Webbook
rinpol	3244.00		NIST Webbook
tb	1088.85	K	Joback Method
tc	1336.67	K	Joback Method
tf	700.22	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1235.00	J/mol×K	1088.85	Joback Method
cpg	1247.80	J/mol×K	1130.15	Joback Method
cpg	1258.85	J/mol×K	1171.46	Joback Method
cpg	1268.21	J/mol×K	1212.76	Joback Method
cpg	1275.94	J/mol×K	1254.07	Joback Method
cpg	1282.11	J/mol×K	1295.37	Joback Method
cpg	1286.78	J/mol×K	1336.67	Joback Method

Sources

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=U380700&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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