Sebacic acid, 2-(3-nitrophenyl)ethyl pentyl ester

Inchi: InChI=1S/C23H35NO6/c1-2-3-10-17-29-22(25)14-8-6-4-5-7-9-15-23(26)30-18-16-20-12-
InchiKey: HVNRVBAIJJPQNA-UHFFFAOYSA-N
Formula: C23H35NO6
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 421.53

Physical Properties

Property code	Value	Unit	Source
gf	-186.73	kJ/mol	Joback Method
hf	-793.35	kJ/mol	Joback Method
hfus	65.91	kJ/mol	Joback Method
hvap	104.63	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.535		Crippen Method
mcvol	343.470	ml/mol	McGowan Method
pc	1106.68	kPa	Joback Method
rinpol	3146.00		NIST Webbook
rinpol	3146.00		NIST Webbook
tb	1061.72	K	Joback Method
tc	1300.03	K	Joback Method
tf	675.84	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.01	J/mol×K	1061.72	Joback Method
cpg	1181.96	J/mol×K	1101.44	Joback Method
cpg	1193.35	J/mol×K	1141.16	Joback Method
cpg	1203.22	J/mol×K	1180.88	Joback Method
cpg	1211.64	J/mol×K	1220.59	Joback Method
cpg	1218.67	J/mol×K	1260.31	Joback Method
cpg	1224.35	J/mol×K	1300.03	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=U380658&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