Sebacic hexyl 3-nitrophenyl ester

Inchi: InChI=1S/C22H33NO6/c1-2-3-4-11-17-28-21(24)15-9-7-5-6-8-10-16-22(25)29-20-14-12-
InchiKey: IHSDHTSHMNWKIS-UHFFFAOYSA-N
Formula: C22H33NO6
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 407.50

Physical Properties

Property code	Value	Unit	Source
gf	-195.15	kJ/mol	Joback Method
hf	-772.71	kJ/mol	Joback Method
hfus	63.32	kJ/mol	Joback Method
hvap	102.41	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	5.744		Crippen Method
mcvol	329.380	ml/mol	McGowan Method
pc	1180.90	kPa	Joback Method
rinpol	3213.00		NIST Webbook
tb	1038.84	K	Joback Method
tc	1271.93	K	Joback Method
tf	664.57	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.40	J/mol×K	1038.84	Joback Method
cpg	1121.22	J/mol×K	1077.69	Joback Method
cpg	1132.57	J/mol×K	1116.54	Joback Method
cpg	1142.47	J/mol×K	1155.39	Joback Method
cpg	1150.99	J/mol×K	1194.23	Joback Method
cpg	1158.17	J/mol×K	1233.08	Joback Method
cpg	1164.06	J/mol×K	1271.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354918&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