Sebacic acid, isohexyl 4-nitrophenyl ester

Inchi: InChI=1S/C22H33NO6/c1-18(2)10-9-17-28-21(24)11-7-5-3-4-6-8-12-22(25)29-20-15-13-
InchiKey: IXAMUZUXGNWKER-UHFFFAOYSA-N
Formula: C22H33NO6
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 407.50

Physical Properties

Property code	Value	Unit	Source
gf	-197.59	kJ/mol	Joback Method
hf	-777.99	kJ/mol	Joback Method
hfus	59.80	kJ/mol	Joback Method
hvap	102.02	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.600		Crippen Method
mcvol	329.380	ml/mol	McGowan Method
pc	1187.42	kPa	Joback Method
rinpol	3211.00		NIST Webbook
tb	1038.40	K	Joback Method
tc	1271.66	K	Joback Method
tf	649.57	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.70	J/mol×K	1038.40	Joback Method
cpg	1121.45	J/mol×K	1077.28	Joback Method
cpg	1132.70	J/mol×K	1116.15	Joback Method
cpg	1142.50	J/mol×K	1155.03	Joback Method
cpg	1150.89	J/mol×K	1193.90	Joback Method
cpg	1157.93	J/mol×K	1232.78	Joback Method
cpg	1163.67	J/mol×K	1271.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354788&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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