Sebacic acid, hexyl 2-methyl-3-nitrobenzyl ester

Inchi: InChI=1S/C24H37NO6/c1-3-4-5-12-18-30-23(26)16-10-8-6-7-9-11-17-24(27)31-19-21-14

InchiKey: HSPIDGNVLDEUAV-UHFFFAOYSA-N

Formula: C24H37NO6

SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCc1cccc([N+](=O)[O-])c1C

Mol. weight [g/mol]: 435.55

Physical Properties

Property code	Value	Unit	Source
gf	-187.94	kJ/mol	Joback Method
hf	-825.46	kJ/mol	Joback Method
hfus	68.11	kJ/mol	Joback Method
hvap	107.52	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	6.191		Crippen Method
mcvol	357.560	ml/mol	McGowan Method
pc	1029.26	kPa	Joback Method
rinpol	3214.00		NIST Webbook
rinpol	3214.00		NIST Webbook
tb	1089.58	K	Joback Method
tc	1335.53	K	Joback Method
tf	699.63	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1228.54	J/mol×K	1089.58	Joback Method
cpg	1241.38	J/mol×K	1130.57	Joback Method
cpg	1252.49	J/mol×K	1171.56	Joback Method
cpg	1261.92	J/mol×K	1212.56	Joback Method
cpg	1269.74	J/mol×K	1253.55	Joback Method
cpg	1276.00	J/mol×K	1294.54	Joback Method
cpg	1280.76	J/mol×K	1335.53	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=U380728&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