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

Inchi: InChI=1S/C23H35NO6/c1-3-4-11-17-29-22(25)15-9-7-5-6-8-10-16-23(26)30-18-20-13-12

InchiKey: UWSFSXCCZIRBPH-UHFFFAOYSA-N

Formula: C23H35NO6

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

Mol. weight [g/mol]: 421.53

Physical Properties

Property code	Value	Unit	Source
gf	-196.36	kJ/mol	Joback Method
hf	-804.82	kJ/mol	Joback Method
hfus	65.52	kJ/mol	Joback Method
hvap	105.30	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	5.801		Crippen Method
mcvol	343.470	ml/mol	McGowan Method
pc	1095.72	kPa	Joback Method
rinpol	3126.00		NIST Webbook
rinpol	3126.00		NIST Webbook
tb	1066.70	K	Joback Method
tc	1306.18	K	Joback Method
tf	688.36	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1167.63	J/mol×K	1066.70	Joback Method
cpg	1180.37	J/mol×K	1106.61	Joback Method
cpg	1191.47	J/mol×K	1146.53	Joback Method
cpg	1201.00	J/mol×K	1186.44	Joback Method
cpg	1209.00	J/mol×K	1226.35	Joback Method
cpg	1215.52	J/mol×K	1266.27	Joback Method
cpg	1220.61	J/mol×K	1306.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380727&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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