Sebacic acid, isobutyl 4-nitrobenzyl ester

Inchi: InChI=1S/C21H31NO6/c1-17(2)15-27-20(23)9-7-5-3-4-6-8-10-21(24)28-16-18-11-13-19(
InchiKey: MPEFIVANZIGVMR-UHFFFAOYSA-N
Formula: C21H31NO6
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 393.47

Physical Properties

Property code	Value	Unit	Source
gf	-206.01	kJ/mol	Joback Method
hf	-757.35	kJ/mol	Joback Method
hfus	57.21	kJ/mol	Joback Method
hvap	99.79	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	4.958		Crippen Method
mcvol	315.290	ml/mol	McGowan Method
pc	1270.06	kPa	Joback Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	1015.52	K	Joback Method
tc	1245.06	K	Joback Method
tf	638.30	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.54	J/mol×K	1015.52	Joback Method
cpg	1061.21	J/mol×K	1053.78	Joback Method
cpg	1072.44	J/mol×K	1092.03	Joback Method
cpg	1082.28	J/mol×K	1130.29	Joback Method
cpg	1090.77	J/mol×K	1168.55	Joback Method
cpg	1097.95	J/mol×K	1206.81	Joback Method
cpg	1103.87	J/mol×K	1245.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380803&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

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