Sebacic acid, isobutyl 4-methoxy-3-nitrobenzyl ester

Inchi: InChI=1S/C22H33NO7/c1-17(2)15-29-21(24)10-8-6-4-5-7-9-11-22(25)30-16-18-12-13-20

InchiKey: NSIKRCRRGOIMTR-UHFFFAOYSA-N

Formula: C22H33NO7

SMILES: COc1ccc(COC(=O)CCCCCCCCC(=O)OCC(C)C)cc1[N+](=O)[O-]

Mol. weight [g/mol]: 423.50

Physical Properties

Property code	Value	Unit	Source
gf	-312.22	kJ/mol	Joback Method
hf	-921.68	kJ/mol	Joback Method
hfus	60.60	kJ/mol	Joback Method
hvap	105.09	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	4.967		Crippen Method
mcvol	335.250	ml/mol	McGowan Method
pc	1161.66	kPa	Joback Method
rinpol	3130.00		NIST Webbook
rinpol	3130.00		NIST Webbook
tb	1065.80	K	Joback Method
tc	1304.85	K	Joback Method
tf	684.32	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1132.64	J/mol×K	1065.80	Joback Method
cpg	1143.89	J/mol×K	1105.64	Joback Method
cpg	1153.32	J/mol×K	1145.48	Joback Method
cpg	1160.96	J/mol×K	1185.33	Joback Method
cpg	1166.83	J/mol×K	1225.17	Joback Method
cpg	1170.96	J/mol×K	1265.01	Joback Method
cpg	1173.36	J/mol×K	1304.85	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=U380649&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