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

Inchi: InChI=1S/C22H33NO6/c1-17(2)15-28-21(24)13-8-6-4-5-7-9-14-22(25)29-16-19-11-10-12

InchiKey: SGYHIYIVDMVKHE-UHFFFAOYSA-N

Formula: C22H33NO6

SMILES: Cc1c(COC(=O)CCCCCCCCC(=O)OCC(C)C)cccc1[N+](=O)[O-]

Mol. weight [g/mol]: 407.50

Physical Properties

Property code	Value	Unit	Source
gf	-207.22	kJ/mol	Joback Method
hf	-789.46	kJ/mol	Joback Method
hfus	59.41	kJ/mol	Joback Method
hvap	102.68	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.266		Crippen Method
mcvol	329.380	ml/mol	McGowan Method
pc	1175.24	kPa	Joback Method
rinpol	3003.00		NIST Webbook
rinpol	3003.00		NIST Webbook
tb	1043.38	K	Joback Method
tc	1277.70	K	Joback Method
tf	662.09	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.35	J/mol×K	1043.38	Joback Method
cpg	1119.92	J/mol×K	1082.43	Joback Method
cpg	1130.92	J/mol×K	1121.49	Joback Method
cpg	1140.42	J/mol×K	1160.54	Joback Method
cpg	1148.44	J/mol×K	1199.59	Joback Method
cpg	1155.04	J/mol×K	1238.64	Joback Method
cpg	1160.25	J/mol×K	1277.70	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=U380725&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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