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

Inchi: InChI=1S/C21H31NO6/c1-3-15-27-20(23)13-8-6-4-5-7-9-14-21(24)28-16-18-11-10-12-19

InchiKey: CCSIPPYCSKYFFW-UHFFFAOYSA-N

Formula: C21H31NO6

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

Mol. weight [g/mol]: 393.47

Physical Properties

Property code	Value	Unit	Source
gf	-213.20	kJ/mol	Joback Method
hf	-763.54	kJ/mol	Joback Method
hfus	60.34	kJ/mol	Joback Method
hvap	100.84	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.020		Crippen Method
mcvol	315.290	ml/mol	McGowan Method
pc	1249.49	kPa	Joback Method
rinpol	2959.00		NIST Webbook
rinpol	2959.00		NIST Webbook
tb	1020.94	K	Joback Method
tc	1250.92	K	Joback Method
tf	665.82	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1046.88	J/mol×K	1020.94	Joback Method
cpg	1059.43	J/mol×K	1059.27	Joback Method
cpg	1070.51	J/mol×K	1097.60	Joback Method
cpg	1080.17	J/mol×K	1135.93	Joback Method
cpg	1088.45	J/mol×K	1174.26	Joback Method
cpg	1095.38	J/mol×K	1212.59	Joback Method
cpg	1100.99	J/mol×K	1250.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380724&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