Sebacic acid, isobutyl 3-nitro-4-chlorobenzyl ester

Inchi: InChI=1S/C21H30ClNO6/c1-16(2)14-28-20(24)9-7-5-3-4-6-8-10-21(25)29-15-17-11-12-1

InchiKey: ZKIIDGLPQQRMJG-UHFFFAOYSA-N

Formula: C21H30ClNO6

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCc1ccc(Cl)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 427.92

Physical Properties

Property code	Value	Unit	Source
gf	-227.57	kJ/mol	Joback Method
hf	-784.56	kJ/mol	Joback Method
hfus	61.02	kJ/mol	Joback Method
hvap	104.84	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	5.611		Crippen Method
mcvol	327.530	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinpol	3073.00		NIST Webbook
rinpol	3073.00		NIST Webbook
tb	1057.93	K	Joback Method
tc	1295.69	K	Joback Method
tf	680.74	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.31	J/mol×K	1057.93	Joback Method
cpg	1078.46	J/mol×K	1097.56	Joback Method
cpg	1088.10	J/mol×K	1137.18	Joback Method
cpg	1096.28	J/mol×K	1176.81	Joback Method
cpg	1103.04	J/mol×K	1216.44	Joback Method
cpg	1108.42	J/mol×K	1256.07	Joback Method
cpg	1112.47	J/mol×K	1295.69	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=U380581&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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