Succinic acid, decyl 4-methoxy-3-nitrobenzyl ester

Inchi: InChI=1S/C22H33NO7/c1-3-4-5-6-7-8-9-10-15-29-21(24)13-14-22(25)30-17-18-11-12-20

InchiKey: AMJVPEKIFIEPFQ-UHFFFAOYSA-N

Formula: C22H33NO7

SMILES: CCCCCCCCCCOC(=O)CCC(=O)OCc1ccc(OC)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 423.50

Physical Properties

Property code	Value	Unit	Source
gf	-309.78	kJ/mol	Joback Method
hf	-916.40	kJ/mol	Joback Method
hfus	64.12	kJ/mol	Joback Method
hvap	105.48	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	5.111		Crippen Method
mcvol	335.250	ml/mol	McGowan Method
pc	1155.35	kPa	Joback Method
rinpol	3212.00		NIST Webbook
rinpol	3212.00		NIST Webbook
tb	1066.24	K	Joback Method
tc	1305.54	K	Joback Method
tf	699.32	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1132.39	J/mol×K	1066.24	Joback Method
cpg	1143.74	J/mol×K	1106.12	Joback Method
cpg	1153.28	J/mol×K	1146.01	Joback Method
cpg	1161.05	J/mol×K	1185.89	Joback Method
cpg	1167.06	J/mol×K	1225.77	Joback Method
cpg	1171.34	J/mol×K	1265.66	Joback Method
cpg	1173.91	J/mol×K	1305.54	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=U380955&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