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

Inchi: InChI=1S/C17H23NO7/c1-3-4-5-10-24-16(19)8-9-17(20)25-12-13-6-7-15(23-2)14(11-13)
InchiKey: WTAMDSWSRSKAAX-UHFFFAOYSA-N
Formula: C17H23NO7
SMILES: CCCCCOC(=O)CCC(=O)OCc1ccc(OC)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 353.37

Physical Properties

Property code	Value	Unit	Source
gf	-351.88	kJ/mol	Joback Method
hf	-813.20	kJ/mol	Joback Method
hfus	51.17	kJ/mol	Joback Method
hvap	94.35	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.160		Crippen Method
mcvol	264.800	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	2727.00		NIST Webbook
rinpol	2727.00		NIST Webbook
tb	951.84	K	Joback Method
tc	1175.57	K	Joback Method
tf	642.97	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.16	J/mol×K	951.84	Joback Method
cpg	848.49	J/mol×K	989.13	Joback Method
cpg	858.45	J/mol×K	1026.42	Joback Method
cpg	867.04	J/mol×K	1063.71	Joback Method
cpg	874.26	J/mol×K	1100.99	Joback Method
cpg	880.11	J/mol×K	1138.28	Joback Method
cpg	884.59	J/mol×K	1175.57	Joback Method

Sources

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=U380950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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