Succinic acid, di(4-methyl-3-nitrobenzyl) ester

Inchi: InChI=1S/C20H20N2O8/c1-13-3-5-15(9-17(13)21(25)26)11-29-19(23)7-8-20(24)30-12-16
InchiKey: KQTLDCWUNXWULN-UHFFFAOYSA-N
Formula: C20H20N2O8
SMILES: Cc1ccc(COC(=O)CCC(=O)OCc2ccc(C)c([N+](=O)[O-])c2)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 416.38

Physical Properties

Property code	Value	Unit	Source
gf	-92.92	kJ/mol	Joback Method
hf	-540.07	kJ/mol	Joback Method
hfus	62.38	kJ/mol	Joback Method
hvap	118.81	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	3.687		Crippen Method
mcvol	294.860	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	3367.00		NIST Webbook
rinpol	3367.00		NIST Webbook
tb	1186.54	K	Joback Method
tc	1456.55	K	Joback Method
tf	849.62	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.92	J/mol×K	1186.54	Joback Method
cpg	950.06	J/mol×K	1231.54	Joback Method
cpg	952.49	J/mol×K	1276.54	Joback Method
cpg	953.25	J/mol×K	1321.54	Joback Method
cpg	952.39	J/mol×K	1366.54	Joback Method
cpg	949.97	J/mol×K	1411.55	Joback Method
cpg	946.04	J/mol×K	1456.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381132&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