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

Inchi: InChI=1S/C14H17NO7/c1-3-21-13(16)6-7-14(17)22-9-10-4-5-12(20-2)11(8-10)15(18)19/
InchiKey: JDHLFBKTGIZWFZ-UHFFFAOYSA-N
Formula: C14H17NO7
SMILES: CCOC(=O)CCC(=O)OCc1ccc(OC)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 311.29

Physical Properties

Property code	Value	Unit	Source
gf	-377.14	kJ/mol	Joback Method
hf	-751.28	kJ/mol	Joback Method
hfus	43.40	kJ/mol	Joback Method
hvap	87.67	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	1.990		Crippen Method
mcvol	222.530	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	2432.00		NIST Webbook
rinpol	2432.00		NIST Webbook
tb	883.20	K	Joback Method
tc	1108.30	K	Joback Method
tf	609.16	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.42	J/mol×K	883.20	Joback Method
cpg	677.45	J/mol×K	920.72	Joback Method
cpg	687.27	J/mol×K	958.23	Joback Method
cpg	695.87	J/mol×K	995.75	Joback Method
cpg	703.24	J/mol×K	1033.27	Joback Method
cpg	709.36	J/mol×K	1070.78	Joback Method
cpg	714.24	J/mol×K	1108.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380947&Units=SI

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