Succinic acid, 4-nitrobenzyl pentyl ester

Inchi: InChI=1S/C16H21NO6/c1-2-3-4-11-22-15(18)9-10-16(19)23-12-13-5-7-14(8-6-13)17(20)
InchiKey: DGPIQTIGKJFASY-UHFFFAOYSA-N
Formula: C16H21NO6
SMILES: CCCCCOC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 323.34

Physical Properties

Property code	Value	Unit	Source
gf	-245.67	kJ/mol	Joback Method
hf	-648.87	kJ/mol	Joback Method
hfus	47.78	kJ/mol	Joback Method
hvap	89.05	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.152		Crippen Method
mcvol	244.840	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
rinpol	2499.00		NIST Webbook
rinpol	2499.00		NIST Webbook
tb	901.56	K	Joback Method
tc	1124.04	K	Joback Method
tf	596.95	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.95	J/mol×K	901.56	Joback Method
cpg	767.04	J/mol×K	938.64	Joback Method
cpg	777.96	J/mol×K	975.72	Joback Method
cpg	787.73	J/mol×K	1012.80	Joback Method
cpg	796.37	J/mol×K	1049.88	Joback Method
cpg	803.89	J/mol×K	1086.96	Joback Method
cpg	810.33	J/mol×K	1124.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381169&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

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