Succinic acid, isobutyl 3-methyl-4-nitrobenzyl ester

Inchi: InChI=1S/C16H21NO6/c1-11(2)9-22-15(18)6-7-16(19)23-10-13-4-5-14(17(20)21)12(3)8-

InchiKey: AYLNQQFQYJFZRM-UHFFFAOYSA-N

Formula: C16H21NO6

SMILES: Cc1cc(COC(=O)CCC(=O)OCC(C)C)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 323.34

Physical Properties

Property code	Value	Unit	Source
gf	-257.74	kJ/mol	Joback Method
hf	-665.62	kJ/mol	Joback Method
hfus	43.87	kJ/mol	Joback Method
hvap	89.33	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	2.926		Crippen Method
mcvol	244.840	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	2399.00		NIST Webbook
rinpol	2399.00		NIST Webbook
tb	906.10	K	Joback Method
tc	1131.81	K	Joback Method
tf	594.47	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.10	J/mol×K	906.10	Joback Method
cpg	766.19	J/mol×K	943.72	Joback Method
cpg	777.05	J/mol×K	981.34	Joback Method
cpg	786.69	J/mol×K	1018.96	Joback Method
cpg	795.14	J/mol×K	1056.57	Joback Method
cpg	802.40	J/mol×K	1094.19	Joback Method
cpg	808.50	J/mol×K	1131.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380979&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