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

Inchi: InChI=1S/C16H21NO7/c1-11(2)9-23-15(18)6-7-16(19)24-10-12-4-5-14(22-3)13(8-12)17(

InchiKey: NLTGQSGRGSRKLB-UHFFFAOYSA-N

Formula: C16H21NO7

SMILES: COc1ccc(COC(=O)CCC(=O)OCC(C)C)cc1[N+](=O)[O-]

Mol. weight [g/mol]: 339.34

Physical Properties

Property code	Value	Unit	Source
gf	-362.74	kJ/mol	Joback Method
hf	-797.84	kJ/mol	Joback Method
hfus	45.06	kJ/mol	Joback Method
hvap	91.73	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.626		Crippen Method
mcvol	250.710	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	928.52	K	Joback Method
tc	1154.05	K	Joback Method
tf	616.70	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.10	J/mol×K	928.52	Joback Method
cpg	791.43	J/mol×K	966.11	Joback Method
cpg	801.41	J/mol×K	1003.70	Joback Method
cpg	810.03	J/mol×K	1041.29	Joback Method
cpg	817.29	J/mol×K	1078.87	Joback Method
cpg	823.19	J/mol×K	1116.46	Joback Method
cpg	827.73	J/mol×K	1154.05	Joback Method

Sources

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=U380948&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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