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

Inchi: InChI=1S/C16H21NO7/c1-3-4-9-23-15(18)7-8-16(19)24-11-12-5-6-13(17(20)21)14(10-12

InchiKey: RBRLBQWIPGQETB-UHFFFAOYSA-N

Formula: C16H21NO7

SMILES: CCCCOC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])c(OC)c1

Mol. weight [g/mol]: 339.34

Physical Properties

Property code	Value	Unit	Source
gf	-360.30	kJ/mol	Joback Method
hf	-792.56	kJ/mol	Joback Method
hfus	48.58	kJ/mol	Joback Method
hvap	92.12	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	2.770		Crippen Method
mcvol	250.710	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2597.00		NIST Webbook
rinpol	2597.00		NIST Webbook
tb	928.96	K	Joback Method
tc	1152.36	K	Joback Method
tf	631.70	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.58	J/mol×K	928.96	Joback Method
cpg	790.85	J/mol×K	966.19	Joback Method
cpg	800.81	J/mol×K	1003.43	Joback Method
cpg	809.44	J/mol×K	1040.66	Joback Method
cpg	816.76	J/mol×K	1077.89	Joback Method
cpg	822.76	J/mol×K	1115.13	Joback Method
cpg	827.43	J/mol×K	1152.36	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=U381012&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