Succinic acid, isobutyl 2-(4-nitrophenoxy)ethyl ester

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

InchiKey: XYYYXFUDPDTQQR-UHFFFAOYSA-N

Formula: C16H21NO7

SMILES: CC(C)COC(=O)CCC(=O)OCCOc1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 339.34

Physical Properties

Property code	Value	Unit	Source
gf	-353.11	kJ/mol	Joback Method
hf	-786.37	kJ/mol	Joback Method
hfus	45.45	kJ/mol	Joback Method
hvap	91.07	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.496		Crippen Method
mcvol	250.710	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	2624.00		NIST Webbook
rinpol	2624.00		NIST Webbook
tb	923.54	K	Joback Method
tc	1148.28	K	Joback Method
tf	604.18	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.56	J/mol×K	923.54	Joback Method
cpg	793.01	J/mol×K	961.00	Joback Method
cpg	803.14	J/mol×K	998.45	Joback Method
cpg	811.93	J/mol×K	1035.91	Joback Method
cpg	819.41	J/mol×K	1073.36	Joback Method
cpg	825.57	J/mol×K	1110.82	Joback Method
cpg	830.42	J/mol×K	1148.28	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=U381134&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