Phthalic acid, 3-methoxy-4-nitrobenzyl propyl ester

Inchi: InChI=1S/C19H19NO7/c1-3-10-26-18(21)14-6-4-5-7-15(14)19(22)27-12-13-8-9-16(20(23

InchiKey: CFVINQBUUWIQAP-UHFFFAOYSA-N

Formula: C19H19NO7

SMILES: CCCOC(=O)c1ccccc1C(=O)OCc1ccc([N+](=O)[O-])c(OC)c1

Mol. weight [g/mol]: 373.36

Physical Properties

Property code	Value	Unit	Source
gf	-232.26	kJ/mol	Joback Method
hf	-629.42	kJ/mol	Joback Method
hfus	50.00	kJ/mol	Joback Method
hvap	101.74	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	3.527		Crippen Method
mcvol	269.220	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	3279.00		NIST Webbook
rinpol	3279.00		NIST Webbook
tb	1029.26	K	Joback Method
tc	1275.28	K	Joback Method
tf	704.45	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.15	J/mol×K	1029.26	Joback Method
cpg	848.55	J/mol×K	1070.26	Joback Method
cpg	855.31	J/mol×K	1111.27	Joback Method
cpg	860.44	J/mol×K	1152.27	Joback Method
cpg	863.96	J/mol×K	1193.27	Joback Method
cpg	865.87	J/mol×K	1234.28	Joback Method
cpg	866.19	J/mol×K	1275.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382530&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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