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

Inchi: InChI=1S/C20H21NO7/c1-13(2)11-27-19(22)15-6-4-5-7-16(15)20(23)28-12-14-8-9-17(21

InchiKey: ICMIQBBNDRPXAC-UHFFFAOYSA-N

Formula: C20H21NO7

SMILES: COc1cc(COC(=O)c2ccccc2C(=O)OCC(C)C)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 387.38

Physical Properties

Property code	Value	Unit	Source
gf	-226.28	kJ/mol	Joback Method
hf	-655.34	kJ/mol	Joback Method
hfus	49.07	kJ/mol	Joback Method
hvap	103.58	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	3.773		Crippen Method
mcvol	283.310	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
rinpol	3343.00		NIST Webbook
rinpol	3343.00		NIST Webbook
tb	1051.70	K	Joback Method
tc	1299.62	K	Joback Method
tf	700.72	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.05	J/mol×K	1051.70	Joback Method
cpg	906.29	J/mol×K	1093.02	Joback Method
cpg	912.81	J/mol×K	1134.34	Joback Method
cpg	917.61	J/mol×K	1175.66	Joback Method
cpg	920.72	J/mol×K	1216.98	Joback Method
cpg	922.16	J/mol×K	1258.30	Joback Method
cpg	921.93	J/mol×K	1299.62	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=U382531&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