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

Inchi: InChI=1S/C24H29NO7/c1-3-4-5-6-7-10-15-31-23(26)19-11-8-9-12-20(19)24(27)32-17-18
InchiKey: MAUKRILGTLHOGK-UHFFFAOYSA-N
Formula: C24H29NO7
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc([N+](=O)[O-])c(OC)c1
Mol. weight [g/mol]: 443.49

Physical Properties

Property code	Value	Unit	Source
gf	-190.16	kJ/mol	Joback Method
hf	-732.62	kJ/mol	Joback Method
hfus	62.95	kJ/mol	Joback Method
hvap	112.87	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	5.478		Crippen Method
mcvol	339.670	ml/mol	McGowan Method
pc	1259.27	kPa	Joback Method
rinpol	3881.00		NIST Webbook
rinpol	3881.00		NIST Webbook
tb	1143.66	K	Joback Method
tc	1400.19	K	Joback Method
tf	760.80	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1131.43	J/mol×K	1143.66	Joback Method
cpg	1138.98	J/mol×K	1186.41	Joback Method
cpg	1144.57	J/mol×K	1229.17	Joback Method
cpg	1148.23	J/mol×K	1271.92	Joback Method
cpg	1150.01	J/mol×K	1314.68	Joback Method
cpg	1149.95	J/mol×K	1357.43	Joback Method
cpg	1148.09	J/mol×K	1400.19	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=U382536&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