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

Inchi: InChI=1S/C21H23NO7/c1-3-4-7-12-28-20(23)16-8-5-6-9-17(16)21(24)29-14-15-10-11-18

InchiKey: NMDVSUSBWNUGCD-UHFFFAOYSA-N

Formula: C21H23NO7

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

Mol. weight [g/mol]: 401.41

Physical Properties

Property code	Value	Unit	Source
gf	-215.42	kJ/mol	Joback Method
hf	-670.70	kJ/mol	Joback Method
hfus	55.18	kJ/mol	Joback Method
hvap	106.19	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	4.307		Crippen Method
mcvol	297.400	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	3588.00		NIST Webbook
rinpol	3588.00		NIST Webbook
tb	1075.02	K	Joback Method
tc	1322.11	K	Joback Method
tf	726.99	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.69	J/mol×K	1075.02	Joback Method
cpg	963.82	J/mol×K	1116.20	Joback Method
cpg	970.21	J/mol×K	1157.38	Joback Method
cpg	974.88	J/mol×K	1198.56	Joback Method
cpg	977.86	J/mol×K	1239.75	Joback Method
cpg	979.17	J/mol×K	1280.93	Joback Method
cpg	978.83	J/mol×K	1322.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382533&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