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

Inchi: InChI=1S/C21H23NO6/c1-3-4-7-12-27-20(23)17-8-5-6-9-18(17)21(24)28-14-16-11-10-15

InchiKey: QXWIOUCPQXLAFS-UHFFFAOYSA-N

Formula: C21H23NO6

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

Mol. weight [g/mol]: 385.41

Physical Properties

Property code	Value	Unit	Source
gf	-110.42	kJ/mol	Joback Method
hf	-538.48	kJ/mol	Joback Method
hfus	54.00	kJ/mol	Joback Method
hvap	103.78	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	4.607		Crippen Method
mcvol	291.530	ml/mol	McGowan Method
pc	1583.49	kPa	Joback Method
rinpol	3258.00		NIST Webbook
rinpol	3258.00		NIST Webbook
tb	1052.60	K	Joback Method
tc	1298.25	K	Joback Method
tf	704.76	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.47	J/mol×K	1052.60	Joback Method
cpg	942.10	J/mol×K	1093.54	Joback Method
cpg	950.22	J/mol×K	1134.48	Joback Method
cpg	956.89	J/mol×K	1175.42	Joback Method
cpg	962.15	J/mol×K	1216.37	Joback Method
cpg	966.03	J/mol×K	1257.31	Joback Method
cpg	968.60	J/mol×K	1298.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382583&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