Phthalic acid, 3,5-dinitro-4-methylbenzyl pentyl ester

Inchi: InChI=1S/C21H22N2O8/c1-3-4-7-10-30-20(24)16-8-5-6-9-17(16)21(25)31-13-15-11-18(2

InchiKey: CGPIVFZHWNZWCV-UHFFFAOYSA-N

Formula: C21H22N2O8

SMILES: CCCCCOC(=O)c1ccccc1C(=O)OCc1cc([N+](=O)[O-])c(C)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 430.41

Physical Properties

Property code	Value	Unit	Source
gf	-84.50	kJ/mol	Joback Method
hf	-560.71	kJ/mol	Joback Method
hfus	64.97	kJ/mol	Joback Method
hvap	121.03	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	4.515		Crippen Method
mcvol	308.950	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	3354.00		NIST Webbook
rinpol	3354.00		NIST Webbook
tb	1209.42	K	Joback Method
tc	1482.07	K	Joback Method
tf	860.89	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.71	J/mol×K	1209.42	Joback Method
cpg	1007.68	J/mol×K	1254.86	Joback Method
cpg	1009.89	J/mol×K	1300.30	Joback Method
cpg	1010.40	J/mol×K	1345.75	Joback Method
cpg	1009.27	J/mol×K	1391.19	Joback Method
cpg	1006.54	J/mol×K	1436.63	Joback Method
cpg	1002.29	J/mol×K	1482.07	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=U415513&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