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

Inchi: InChI=1S/C22H24N2O8/c1-3-4-5-8-11-31-21(25)17-9-6-7-10-18(17)22(26)32-14-16-12-1

InchiKey: IKJWEOPPINDGJN-UHFFFAOYSA-N

Formula: C22H24N2O8

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

Mol. weight [g/mol]: 444.43

Physical Properties

Property code	Value	Unit	Source
gf	-76.08	kJ/mol	Joback Method
hf	-581.35	kJ/mol	Joback Method
hfus	67.56	kJ/mol	Joback Method
hvap	123.26	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	4.906		Crippen Method
mcvol	323.040	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	2497.00		NIST Webbook
rinpol	2497.00		NIST Webbook
tb	1232.30	K	Joback Method
tc	1508.83	K	Joback Method
tf	872.16	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1061.75	J/mol×K	1232.30	Joback Method
cpg	1065.54	J/mol×K	1278.39	Joback Method
cpg	1067.51	J/mol×K	1324.48	Joback Method
cpg	1067.73	J/mol×K	1370.56	Joback Method
cpg	1066.26	J/mol×K	1416.65	Joback Method
cpg	1063.18	J/mol×K	1462.74	Joback Method
cpg	1058.55	J/mol×K	1508.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415514&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