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

Inchi: InChI=1S/C23H26N2O8/c1-3-4-5-6-9-12-32-22(26)18-10-7-8-11-19(18)23(27)33-15-17-1

InchiKey: SDLCYSOEPDRZQE-UHFFFAOYSA-N

Formula: C23H26N2O8

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

Mol. weight [g/mol]: 458.46

Physical Properties

Property code	Value	Unit	Source
gf	-67.66	kJ/mol	Joback Method
hf	-601.99	kJ/mol	Joback Method
hfus	70.15	kJ/mol	Joback Method
hvap	125.49	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	5.296		Crippen Method
mcvol	337.130	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
tb	1255.18	K	Joback Method
tc	1536.88	K	Joback Method
tf	883.43	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.02	J/mol×K	1255.18	Joback Method
cpg	1123.61	J/mol×K	1302.13	Joback Method
cpg	1125.30	J/mol×K	1349.08	Joback Method
cpg	1125.19	J/mol×K	1396.03	Joback Method
cpg	1123.35	J/mol×K	1442.98	Joback Method
cpg	1119.87	J/mol×K	1489.93	Joback Method
cpg	1114.80	J/mol×K	1536.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415515&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume