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

Inchi: InChI=1S/C19H18N2O8/c1-3-8-28-18(22)14-6-4-5-7-15(14)19(23)29-11-13-9-16(20(24)2
InchiKey: ZUNYYKSSZDXARE-UHFFFAOYSA-N
Formula: C19H18N2O8
SMILES: CCCOC(=O)c1ccccc1C(=O)OCc1cc([N+](=O)[O-])c(C)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 402.35

Physical Properties

Property code	Value	Unit	Source
gf	-101.34	kJ/mol	Joback Method
hf	-519.43	kJ/mol	Joback Method
hfus	59.79	kJ/mol	Joback Method
hvap	116.58	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	3.735		Crippen Method
mcvol	280.770	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	3079.00		NIST Webbook
rinpol	3079.00		NIST Webbook
tb	1163.66	K	Joback Method
tc	1432.19	K	Joback Method
tf	838.35	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.42	J/mol×K	1163.66	Joback Method
cpg	892.70	J/mol×K	1208.42	Joback Method
cpg	895.31	J/mol×K	1253.17	Joback Method
cpg	896.28	J/mol×K	1297.93	Joback Method
cpg	895.66	J/mol×K	1342.68	Joback Method
cpg	893.50	J/mol×K	1387.44	Joback Method
cpg	889.83	J/mol×K	1432.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415510&Units=SI

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

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