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

Inchi: InChI=1S/C20H20N2O8/c1-12(2)10-29-19(23)15-6-4-5-7-16(15)20(24)30-11-14-8-17(21(

InchiKey: XEGIRSRSIWHGRS-UHFFFAOYSA-N

Formula: C20H20N2O8

SMILES: Cc1c([N+](=O)[O-])cc(COC(=O)c2ccccc2C(=O)OCC(C)C)cc1[N+](=O)[O-]

Mol. weight [g/mol]: 416.38

Physical Properties

Property code	Value	Unit	Source
gf	-95.36	kJ/mol	Joback Method
hf	-545.35	kJ/mol	Joback Method
hfus	58.85	kJ/mol	Joback Method
hvap	118.42	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	3.981		Crippen Method
mcvol	294.860	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	3168.00		NIST Webbook
rinpol	3168.00		NIST Webbook
tb	1186.10	K	Joback Method
tc	1457.32	K	Joback Method
tf	834.62	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.88	J/mol×K	1186.10	Joback Method
cpg	949.87	J/mol×K	1231.30	Joback Method
cpg	952.10	J/mol×K	1276.51	Joback Method
cpg	952.64	J/mol×K	1321.71	Joback Method
cpg	951.53	J/mol×K	1366.91	Joback Method
cpg	948.82	J/mol×K	1412.12	Joback Method
cpg	944.56	J/mol×K	1457.32	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=U415511&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