2-Isopropyl-4,6-dinitro-5-methyl phenol

Other names: 2,6-dinitrothymol
Inchi: InChI=1S/C10H12N2O5/c1-5(2)7-4-8(11(14)15)6(3)9(10(7)13)12(16)17/h4-5,13H,1-3H3
InchiKey: XBCVBHKJVWVNID-UHFFFAOYSA-N
Formula: C10H12N2O5
SMILES: Cc1c([N+](=O)[O-])cc(C(C)C)c(O)c1[N+](=O)[O-]
Mol. weight [g/mol]: 240.21
CAS: 303-21-9

Physical Properties

Property code	Value	Unit	Source
gf	30.88	kJ/mol	Joback Method
hf	-251.72	kJ/mol	Joback Method
hfus	39.51	kJ/mol	Joback Method
hvap	87.92	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	2.640		Crippen Method
mcvol	168.710	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
tb	853.68	K	Joback Method
tc	1119.35	K	Joback Method
tf	650.38	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.27	J/mol×K	853.68	Joback Method
cpg	500.07	J/mol×K	897.96	Joback Method
cpg	510.31	J/mol×K	942.24	Joback Method
cpg	520.10	J/mol×K	986.51	Joback Method
cpg	529.56	J/mol×K	1030.79	Joback Method
cpg	538.81	J/mol×K	1075.07	Joback Method
cpg	547.98	J/mol×K	1119.35	Joback Method

Sources

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=C303219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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