4-Sec-butyl-2,6-dinitrophenol

Inchi: InChI=1S/C10H12N2O5/c1-3-6(2)7-4-8(11(14)15)10(13)9(5-7)12(16)17/h4-6,13H,3H2,1-
InchiKey: WJRXGXYMRWUFQF-UHFFFAOYSA-N
Formula: C10H12N2O5
SMILES: CCC(C)c1cc([N+](=O)[O-])c(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 240.21
CAS: 4097-48-7

Physical Properties

Property code	Value	Unit	Source
gf	40.51	kJ/mol	Joback Method
hf	-240.25	kJ/mol	Joback Method
hfus	39.90	kJ/mol	Joback Method
hvap	87.26	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	2.722		Crippen Method
mcvol	168.710	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	848.70	K	Joback Method
tc	1113.71	K	Joback Method
tf	637.86	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.13	J/mol×K	848.70	Joback Method
cpg	501.95	J/mol×K	892.87	Joback Method
cpg	512.19	J/mol×K	937.04	Joback Method
cpg	521.99	J/mol×K	981.20	Joback Method
cpg	531.46	J/mol×K	1025.37	Joback Method
cpg	540.76	J/mol×K	1069.54	Joback Method
cpg	550.00	J/mol×K	1113.71	Joback Method

Sources

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=C4097487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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