2-tert-Butyl-4,6-dinitrophenyl acetate

Other names: 2-tert-Butyl-4,6-dinitro-phenol acetate
Inchi: InChI=1S/C12H14N2O6/c1-7(15)20-11-9(12(2,3)4)5-8(13(16)17)6-10(11)14(18)19/h5-6H
InchiKey: BMJYKXALMDAIEG-UHFFFAOYSA-N
Formula: C12H14N2O6
SMILES: CC(=O)Oc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1C(C)(C)C
Mol. weight [g/mol]: 282.25

Physical Properties

Property code	Value	Unit	Source
gf	-26.30	kJ/mol	Joback Method
hf	-363.96	kJ/mol	Joback Method
hfus	37.80	kJ/mol	Joback Method
hvap	87.61	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	2.726		Crippen Method
mcvol	198.460	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	1943.00		NIST Webbook
tb	892.32	K	Joback Method
tc	1150.86	K	Joback Method
tf	650.78	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.06	J/mol×K	892.32	Joback Method
cpg	598.54	J/mol×K	935.41	Joback Method
cpg	607.92	J/mol×K	978.50	Joback Method
cpg	616.29	J/mol×K	1021.59	Joback Method
cpg	623.68	J/mol×K	1064.68	Joback Method
cpg	630.18	J/mol×K	1107.77	Joback Method
cpg	635.84	J/mol×K	1150.86	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=U373331&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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