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

Other names: 2-(2-Methyl-2-propanyl)-4,6-dinitrophenol trifluoroacetate
Inchi: InChI=1S/C12H11F3N2O6/c1-11(2,3)7-4-6(16(19)20)5-8(17(21)22)9(7)23-10(18)12(13,1
InchiKey: UQRRKBGUXKHVFL-UHFFFAOYSA-N
Formula: C12H11F3N2O6
SMILES: CC(C)(C)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 336.22

Physical Properties

Property code	Value	Unit	Source
gf	-607.89	kJ/mol	Joback Method
hf	-961.04	kJ/mol	Joback Method
hfus	39.63	kJ/mol	Joback Method
hvap	83.86	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.268		Crippen Method
mcvol	203.770	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1692.00		NIST Webbook
rinpol	1692.00		NIST Webbook
tb	886.90	K	Joback Method
tc	1129.48	K	Joback Method
tf	654.97	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.46	J/mol×K	886.90	Joback Method
cpg	620.61	J/mol×K	927.33	Joback Method
cpg	628.88	J/mol×K	967.76	Joback Method
cpg	636.35	J/mol×K	1008.19	Joback Method
cpg	643.12	J/mol×K	1048.62	Joback Method
cpg	649.26	J/mol×K	1089.05	Joback Method
cpg	654.86	J/mol×K	1129.48	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=U373471&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume