4,6-Dinitro-o-cresol, isoBOC

Inchi: InChI=1S/C12H14N2O7/c1-7(2)6-20-12(15)21-11-8(3)4-9(13(16)17)5-10(11)14(18)19/h4
InchiKey: TXXIVECIVKIRBG-UHFFFAOYSA-N
Formula: C12H14N2O7
SMILES: Cc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1OC(=O)OCC(C)C
Mol. weight [g/mol]: 298.25

Physical Properties

Property code	Value	Unit	Source
gf	-136.58	kJ/mol	Joback Method
hf	-492.71	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	90.93	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	2.983		Crippen Method
mcvol	204.330	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	917.53	K	Joback Method
tc	1165.68	K	Joback Method
tf	655.59	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.73	J/mol×K	917.53	Joback Method
cpg	621.42	J/mol×K	958.89	Joback Method
cpg	629.84	J/mol×K	1000.25	Joback Method
cpg	636.99	J/mol×K	1041.61	Joback Method
cpg	642.89	J/mol×K	1082.96	Joback Method
cpg	647.52	J/mol×K	1124.32	Joback Method
cpg	650.88	J/mol×K	1165.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235153&Units=SI
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

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