Benzenemethanol, 2,4,6-trinitro-

Other names: 2,4,6-Trinitrobenzyl alcohol
Inchi: InChI=1S/C7H5N3O7/c11-3-5-6(9(14)15)1-4(8(12)13)2-7(5)10(16)17/h1-2,11H,3H2
InchiKey: IFNVWRBEJGYFNL-UHFFFAOYSA-N
Formula: C7H5N3O7
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c(CO)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 243.13
CAS: 24577-68-2

Physical Properties

Property code	Value	Unit	Source
gf	61.41	kJ/mol	Joback Method
hf	-170.20	kJ/mol	Joback Method
hfus	44.93	kJ/mol	Joback Method
hvap	101.89	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	0.903		Crippen Method
mcvol	143.860	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
tb	948.88	K	Joback Method
tc	1212.39	K	Joback Method
tf	724.28	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.86	J/mol×K	948.88	Joback Method
cpg	409.35	J/mol×K	992.80	Joback Method
cpg	414.15	J/mol×K	1036.72	Joback Method
cpg	418.31	J/mol×K	1080.63	Joback Method
cpg	421.87	J/mol×K	1124.55	Joback Method
cpg	424.89	J/mol×K	1168.47	Joback Method
cpg	427.41	J/mol×K	1212.39	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=C24577682&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume