Toluene, 3-fluoro-4,6-dinitro-

Inchi: InChI=1S/C7H5FN2O4/c1-4-2-5(8)7(10(13)14)3-6(4)9(11)12/h2-3H,1H3
InchiKey: CMIMRMOSIVTUAA-UHFFFAOYSA-N
Formula: C7H5FN2O4
SMILES: Cc1cc(F)c([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 200.12
CAS: 349-01-9

Physical Properties

Property code	Value	Unit	Source
gf	-32.13	kJ/mol	Joback Method
hf	-203.32	kJ/mol	Joback Method
hfus	32.56	kJ/mol	Joback Method
hvap	67.80	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	1.951		Crippen Method
mcvol	122.340	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	704.13	K	Joback Method
tc	965.87	K	Joback Method
tf	520.44	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.66	J/mol×K	704.13	Joback Method
cpg	314.67	J/mol×K	747.75	Joback Method
cpg	322.90	J/mol×K	791.38	Joback Method
cpg	330.36	J/mol×K	835.00	Joback Method
cpg	337.10	J/mol×K	878.62	Joback Method
cpg	343.16	J/mol×K	922.25	Joback Method
cpg	348.56	J/mol×K	965.87	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=C349019&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