2,5-Dinitrofluorene

Other names: Fluorene, 2,5-dinitro-
9H-Fluorene, 2,5-dinitro-
2,5-Dinitro-9H-fluorene
Inchi: InChI=1S/C13H8N2O4/c16-14(17)10-4-5-11-9(7-10)6-8-2-1-3-12(13(8)11)15(18)19/h1-5,
InchiKey: XHAHNUAISBGLEX-UHFFFAOYSA-N
Formula: C13H8N2O4
SMILES: O=[N+]([O-])c1ccc2c(c1)Cc1cccc([N+](=O)[O-])c1-2
Mol. weight [g/mol]: 256.21
CAS: 15110-74-4

Physical Properties

Property code	Value	Unit	Source
gf	408.64	kJ/mol	Joback Method
hf	199.47	kJ/mol	Joback Method
hfus	39.94	kJ/mol	Joback Method
hvap	84.79	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	3.074		Crippen Method
mcvol	170.490	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	430.32		NIST Webbook
rinpol	430.32		NIST Webbook
tb	876.67	K	Joback Method
tc	1162.30	K	Joback Method
tf	655.63	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.18	J/mol×K	876.67	Joback Method
cpg	487.43	J/mol×K	924.27	Joback Method
cpg	497.17	J/mol×K	971.88	Joback Method
cpg	506.63	J/mol×K	1019.48	Joback Method

cpg	515.99	J/mol×K	1067.09	Joback Method
cpg	525.49	J/mol×K	1114.69	Joback Method
cpg	535.31	J/mol×K	1162.30	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=C15110744&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