(Dinitromethyl)benzene

Inchi: InChI=1S/C7H6N2O4/c10-8(11)7(9(12)13)6-4-2-1-3-5-6/h1-5,7H
InchiKey: VMMLSJNPNVTYMN-UHFFFAOYSA-N
Formula: C7H6N2O4
SMILES: O=[N+]([O-])C(c1ccccc1)[N+](=O)[O-]
Mol. weight [g/mol]: 182.13
CAS: 611-38-1

Physical Properties

Property code	Value	Unit	Source
chs	-3571.00 ± 5.90	kJ/mol	NIST Webbook
gf	189.13	kJ/mol	Joback Method
hf	35.00 ± 6.70	kJ/mol	NIST Webbook
hfs	-41.00 ± 5.90	kJ/mol	NIST Webbook
hfus	27.13	kJ/mol	Joback Method
hsub	76.10 ± 0.80	kJ/mol	NIST Webbook
hvap	66.25	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	1.239		Crippen Method
mcvol	120.570	ml/mol	McGowan Method
pc	4288.66	kPa	Joback Method
tb	689.48	K	Joback Method
tc	968.07	K	Joback Method
tf	467.29	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.93	J/mol×K	689.48	Joback Method
cpg	314.21	J/mol×K	735.91	Joback Method
cpg	323.43	J/mol×K	782.34	Joback Method
cpg	331.68	J/mol×K	828.78	Joback Method
cpg	339.02	J/mol×K	875.21	Joback Method
cpg	345.55	J/mol×K	921.64	Joback Method

cpg	351.34	J/mol×K	968.07	Joback Method
hsubt	76.10	kJ/mol	317.50	NIST Webbook

Sources

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=C611381&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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