2,4-Dinitrophenylacetic acid

Other names: Acetic acid, 2,4-dinitrophenyl-
Inchi: InChI=1S/C8H6N2O6/c11-8(12)3-5-1-2-6(9(13)14)4-7(5)10(15)16/h1-2,4H,3H2,(H,11,12)
InchiKey: KCNISYPADDTFDO-UHFFFAOYSA-N
Formula: C8H6N2O6
SMILES: O=C(O)Cc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 226.14
CAS: 643-43-6

Physical Properties

Property code	Value	Unit	Source
gf	-85.01	kJ/mol	Joback Method
hf	-281.19	kJ/mol	Joback Method
hfus	38.15	kJ/mol	Joback Method
hvap	93.61	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	1.130		Crippen Method
mcvol	142.100	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
tb	868.81	K	Joback Method
tc	1116.50	K	Joback Method
tf	629.35	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.01	J/mol×K	868.81	Joback Method
cpg	395.60	J/mol×K	910.09	Joback Method
cpg	401.49	J/mol×K	951.37	Joback Method
cpg	406.73	J/mol×K	992.66	Joback Method
cpg	411.36	J/mol×K	1033.94	Joback Method
cpg	415.43	J/mol×K	1075.22	Joback Method
cpg	418.96	J/mol×K	1116.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C643436&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume