2-methyl-3,5-dinitrobenzamide

Other names:	3,5-dinitro-2-methylbenzamide
	3,5-dinitro-o-toluamide
	3,5-dinitro-ortho-toluamide
	Dinitolmide
Inchi:	InChI=1S/C8H7N3O5/c1-4-6(8(9)12)2-5(10(13)14)3-7(4)11(15)16/h2-3H,1H3,(H2,9,12)
InchiKey:	ZEFNOZRLAWVAQF-UHFFFAOYSA-N
Formula:	C8H7N3O5
SMILES:	Cc1c(C(N)=O)cc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	225.16

Physical Properties

Property code	Value	Unit	Source
hf	-132.83	kJ/mol	Cheméo Relay (1.0)
hfus	38.87	kJ/mol	Joback Method
hvap	90.64	kJ/mol	Cheméo Relay (1.0)
ie	10.10	eV	Cheméo Relay (1.0)
log10ws	-2.84		Cheméo Relay (1.0)
logp	0.910		Crippen Method
mcvol	146.210	ml/mol	McGowan Method
tb	572.16	K	Cheméo Relay (1.0)
tf	425.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.68	J/mol×K	854.14	Joback Method
cpg	407.61	J/mol×K	899.90	Joback Method
cpg	414.64	J/mol×K	945.67	Joback Method
cpg	420.80	J/mol×K	991.43	Joback Method
cpg	426.14	J/mol×K	1037.19	Joback Method
cpg	430.70	J/mol×K	1082.96	Joback Method
cpg	434.53	J/mol×K	1128.72	Joback Method

Sources

Cheméo Relay (1.0, beta):

Equilibrium solubility of dinitolmide in several neat solvents and binary aqueous co-solvent mixtures: Experimental determination and thermodynamic analysis:	https://www.doi.org/10.1016/j.jct.2019.01.013
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point