3,5-Dinitrobenzamide

Other names:	Nitromide
	Benzamide, 3,5-dinitro-
	component of Tristat
	component of Unistat
	component of Unistat-3
	Tristat
	Unistat
Inchi:	InChI=1S/C7H5N3O5/c8-7(11)4-1-5(9(12)13)3-6(2-4)10(14)15/h1-3H,(H2,8,11)
InchiKey:	UUKWKUSGGZNXGA-UHFFFAOYSA-N
Formula:	C7H5N3O5
SMILES:	NC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	211.13
CAS:	121-81-3

Physical Properties

Property code	Value	Unit	Source
gf	109.84	kJ/mol	Joback Method
hf	-74.53	kJ/mol	Joback Method
hfus	36.67	kJ/mol	Joback Method
hvap	85.34	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	0.602		Crippen Method
mcvol	132.120	ml/mol	McGowan Method
pc	4789.21	kPa	Joback Method
tb	826.28	K	Joback Method
tc	1106.99	K	Joback Method
tf	640.52	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.35	J/mol×K	826.28	Joback Method
cpg	357.69	J/mol×K	873.06	Joback Method

cpg	364.14	J/mol×K	919.85	Joback Method
cpg	369.77	J/mol×K	966.63	Joback Method
cpg	374.63	J/mol×K	1013.42	Joback Method
cpg	378.76	J/mol×K	1060.20	Joback Method
cpg	382.24	J/mol×K	1106.99	Joback Method

Sources

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=C121813&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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