Thiocyanic acid, 2,4-dinitrophenyl ester

Other names:	DNRB
	Gryzbol
	Grzybol
	Nirit
	Nirit Supra
	Rhodandinitrobenzol
	Rodatox 60
	RDNB
	2,4-Dinitrophenyl thiocyanate
	2,4-Dinitrothiocyanatobenzene
	2317-W
	Thiocyano-2,4-dinitrobenzene
	DNTB
	Nitrite
	Tri-Rodazene
	Trirodazeen
	2,4-Dinitro-1-thiocyanobenzene
	2,4-Dinitrothiocyanobenzene
	2,4-Dinitrofenylthiokyanat
	2,4-Dinitro-rhodanbenzol
	NBT
	NBT (pesticide)
	NSC 540
	2,4-Dinitro-1-thiocyanato-benzene
Inchi:	InChI=1S/C7H3N3O4S/c8-4-15-7-2-1-5(9(11)12)3-6(7)10(13)14/h1-3H
InchiKey:	XQDQRCRASHAZBA-UHFFFAOYSA-N
Formula:	C7H3N3O4S
SMILES:	N#CSc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	225.18
CAS:	1594-56-5

Physical Properties

Property code	Value	Unit	Source
gf	338.61	kJ/mol	Joback Method
hf	211.01	kJ/mol	Joback Method
hfus	35.51	kJ/mol	Joback Method

hvap	85.25	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.076		Crippen Method
mcvol	138.300	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
rinpol	1925.00		NIST Webbook
tb	870.74	K	Joback Method
tc	1167.22	K	Joback Method
tf	606.72	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.96	J/mol×K	870.74	Joback Method
cpg	343.84	J/mol×K	920.15	Joback Method
cpg	348.79	J/mol×K	969.57	Joback Method
cpg	352.84	J/mol×K	1018.98	Joback Method
cpg	356.03	J/mol×K	1068.39	Joback Method
cpg	358.40	J/mol×K	1117.80	Joback Method
cpg	359.98	J/mol×K	1167.22	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1594565&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume