

2,6-DINITROBENZONITRILE

Inchi: InChI=1S/C7H3N3O4/c8-4-5-6(9(11)12)2-1-3-7(5)10(13)14/h1-3H
InchiKey: ZYDGHQSJZAFMLU-UHFFFAOYSA-N
Formula: C7H3N3O4
SMILES: N#Cc1c([N+](=O)[O-])cccc1[N+](=O)[O-]
Mol. weight [g/mol]: 193.12

Physical Properties

Property code	Value	Unit	Source
hf	217.66	kJ/mol	Cheméo Relay (1.0)
hfus	31.38	kJ/mol	Joback Method
hvap	79.32	kJ/mol	Cheméo Relay (1.0)
ie	10.67	eV	Cheméo Relay (1.0)
log10ws	-3.36		Cheméo Relay (1.0)
logp	1.375		Crippen Method
mcvol	121.950	ml/mol	McGowan Method
tb	571.35	K	Cheméo Relay (1.0)
tf	413.52	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.41	J/mol×K	801.96	Joback Method
cpg	308.14	J/mol×K	849.04	Joback Method
cpg	314.11	J/mol×K	896.12	Joback Method
cpg	319.35	J/mol×K	943.19	Joback Method
cpg	323.93	J/mol×K	990.27	Joback Method
cpg	327.90	J/mol×K	1037.35	Joback Method
cpg	331.29	J/mol×K	1084.43	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35213004&Units=SI
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

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

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