

2-Methoxy-1,3,5-trinitrobenzene

Inchi:	InChI=1S/C7H5N3O7/c1-17-7-5(9(13)14)2-4(8(11)12)3-6(7)10(15)16/h2-3H,1H3
InchiKey:	FMXDVBRYDYFVGS-UHFFFAOYSA-N
Formula:	C7H5N3O7
SMILES:	COc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	243.13
CAS:	606-35-9

Physical Properties

Property code	Value	Unit	Source
hf	-24.33	kJ/mol	Cheméo Relay (1.0)
hfus	42.03	kJ/mol	Joback Method
hvap	86.86	kJ/mol	Cheméo Relay (1.0)
ie	10.03	eV	Cheméo Relay (1.0)
log10ws	-3.12		Cheméo Relay (1.0)
logp	1.420		Crippen Method
mcvol	143.860	ml/mol	McGowan Method
tb	555.46	K	Cheméo Relay (1.0)
tf	342.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	4.74900e+01
Coeff. B	6.46300e-01
Coeff. C	-3.11280e-04
Coeff. D	2.75000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting
Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

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

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