

2-bromo-4,6-dinitroaniline

Inchi:	InChI=1S/C6H4BrN3O4/c7-4-1-3(9(11)12)2-5(6(4)8)10(13)14/h1-2H,8H2
InchiKey:	KWMDHCLJYMBVNS-UHFFFAOYSA-N
Formula:	C6H4BrN3O4
SMILES:	Nc1c(Br)cc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	262.02
CAS:	1817-73-8

Physical Properties

Property code	Value	Unit	Source
hf	115.19	kJ/mol	Cheméo Relay (1.0)
hfus	37.37	kJ/mol	Joback Method
hvap	86.84	kJ/mol	Cheméo Relay (1.0)
ie	9.10	eV	Cheméo Relay (1.0)
log10ws	-3.74		Cheméo Relay (1.0)
logp	1.848		Crippen Method
mcvol	133.960	ml/mol	McGowan Method
tb	584.83	K	Cheméo Relay (1.0)
tf	425.90	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	3.20900e+01
Coeff. B	6.15220e-01
Coeff. C	-4.04280e-04
Coeff. D	9.57000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Sources

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):

Cheméo Relay (1.0, beta):

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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