

BENZOFURAN-2-ONE, 4-AMINO-2,3-DIHYDRO-

Inchi:	InChI=1S/C8H7NO2/c9-6-2-1-3-7-5(6)4-8(10)11-7/h1-3H,4,9H2
InchiKey:	YOFBHFZFSNSGS-UHFFFAOYSA-N
Formula:	C8H7NO2
SMILES:	<chem>Nc1cccc2c1CC(=O)O2</chem>
Mol. weight [g/mol]:	149.15

Physical Properties

Property code	Value	Unit	Source
hfus	19.49	kJ/mol	Joback Method
logp	0.730		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
tb	594.45	K	Cheméo Relay (1.0)
tf	419.02	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.57	J/mol×K	597.79	Joback Method
cpg	268.87	J/mol×K	640.59	Joback Method
cpg	279.37	J/mol×K	683.39	Joback Method
cpg	289.08	J/mol×K	726.19	Joback Method
cpg	298.05	J/mol×K	768.99	Joback Method
cpg	306.31	J/mol×K	811.80	Joback Method
cpg	313.90	J/mol×K	854.60	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C75990997&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>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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