

(+)-5-BROMO-2'-DEOXYURIDINE

Other names:	2'-Deoxy-5-bromouridine
	5-Bdu
	5-Bromo-2'-deoxyuridine
	5-Bromo-2-deoxyuridine
	5-Bromodeoxyuridine
	5-Bromodesoxyuridine
	5-Bromouracil deoxyriboside
	5-Bromouracil-2-deoxyriboside
	5-Budr
	BDU
	BRDU
	BUdR
	Bromodeoxyuridine
	Bromoouridine
	Bromouracil deoxyriboside
	Brudr
	NSC 38297
	Radibud
	Uridine, 5-bromo-2'-deoxy-
Inchi:	InChI=1S/C9H11BrN2O5/c10-4-2-12(9(16)11-8(4)15)7-1-5(14)6(3-13)17-7/h2,5-7,13-14H
InchiKey:	WOVKYSAHUYNMNH-UHFFFAOYSA-N
Formula:	C9H11BrN2O5
SMILES:	O=c1[nH]c(=O)n(C2CC(O)C(CO)O2)cc1Br
Mol. weight [g/mol]:	307.10

Physical Properties

Property code	Value	Unit	Source
logp	-1.542		Crippen Method
mcvol	169.860	ml/mol	McGowan Method
tf	464.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cps	260.65	J/mol×K	298.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	263.37	J/mol×K	303.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	266.08	J/mol×K	308.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	268.80	J/mol×K	313.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	271.51	J/mol×K	318.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	274.23	J/mol×K	323.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	276.94	J/mol×K	328.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	279.66	J/mol×K	333.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	282.38	J/mol×K	338.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	285.09	J/mol×K	343.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	287.81	J/mol×K	348.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	290.52	J/mol×K	353.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine

cps	293.24	J/mol×K	358.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	295.95	J/mol×K	363.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine
cps	298.66	J/mol×K	368.15	Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Molar Heat Capacities of Some Derivatives of Uridine and 2'-Deoxyuridine:

<https://www.doi.org/10.1021/je800243y>

McGowan Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C59143&Units=SI>

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cps: Solid phase heat capacity

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point

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