

3,4,5,6-TETRABROMOPHTHALIMIDE

Other names:	1H-Isoindole-1,3(2H)-dione, 4,5,6,7-tetrabromo-Phthalimide, 3,4,5,6-tetrabromo-3,4,5,6-Tetrabromophthalimide
Inchi:	InChI=1S/C8HBr4NO2/c9-3-1-2(8(15)13-7(1)14)4(10)6(12)5(3)11/h(H,13,14,15)
InchiKey:	QRFTXHFUNIFHST-UHFFFAOYSA-N
Formula:	C8HBr4NO2
SMILES:	O=C1NC(=O)c2c(Br)c(Br)c(Br)c(Br)c21
Mol. weight [g/mol]:	462.72

Physical Properties

Property code	Value	Unit	Source
hfus	35.39	kJ/mol	Joback Method
logp	3.620		Crippen Method
mcvol	172.080	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.18	J/mol×K	894.26	Joback Method
cpg	331.48	J/mol×K	946.11	Joback Method
cpg	336.97	J/mol×K	997.96	Joback Method
cpg	341.66	J/mol×K	1049.82	Joback Method
cpg	345.53	J/mol×K	1101.67	Joback Method
cpg	348.58	J/mol×K	1153.52	Joback Method
cpg	350.80	J/mol×K	1205.37	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C24407327&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

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