

2,4-DIBROMO-1-NAPHTHOL

Other names:	1-Naphthalenol, 2,4-dibromo-
Inchi:	InChI=1S/C10H6Br2O/c11-8-5-9(12)10(13)7-4-2-1-3-6(7)8/h1-5,13H
InchiKey:	PSGUDVJPEWTBRM-UHFFFAOYSA-N
Formula:	C10H6Br2O
SMILES:	Oc1c(Br)cc(Br)c2ccccc12
Mol. weight [g/mol]:	301.96

Physical Properties

Property code	Value	Unit	Source
hf	31.57	kJ/mol	Cheméo Relay (1.0)
hfus	28.29	kJ/mol	Joback Method
log10ws	-4.63		Cheméo Relay (1.0)
logp	4.070		Crippen Method
mcvol	149.410	ml/mol	McGowan Method
tf	387.38	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.58	J/mol×K	696.76	Joback Method
cpg	318.91	J/mol×K	743.10	Joback Method
cpg	326.66	J/mol×K	789.43	Joback Method
cpg	334.03	J/mol×K	835.77	Joback Method
cpg	341.25	J/mol×K	882.10	Joback Method
cpg	348.53	J/mol×K	928.44	Joback Method
cpg	356.09	J/mol×K	974.78	Joback Method
dvisc	0.0002827	Pa×s	517.94	Joback Method
dvisc	0.0001863	Pa×s	547.74	Joback Method
dvisc	0.0001282	Pa×s	577.55	Joback Method
dvisc	0.0000915	Pa×s	607.35	Joback Method
dvisc	0.0000674	Pa×s	637.15	Joback Method
dvisc	0.0000511	Pa×s	666.96	Joback Method
dvisc	0.0000396	Pa×s	696.76	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050499&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
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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