

Benzamide, N-(1-naphthyl)-4-bromo-

Other names:	4-Bromo-N-(1-naphthyl)benzamide Benzamide, N-(1-naphthyl)-4-bromo- Benzamide, p-bromo-N-1-naphthyl-
Inchi:	InChI=1S/C17H12BrNO/c18-14-10-8-13(9-11-14)17(20)19-16-7-3-5-12-4-1-2-6-15(12)16
InchiKey:	HRRXXGCANBDDNQ-UHFFFAOYSA-N
Formula:	C17H12BrNO
SMILES:	O=C(Nc1cccc2ccccc12)c1ccc(Br)cc1
Mol. weight [g/mol]:	326.19

Physical Properties

Property code	Value	Unit	Source
hf	100.01	kJ/mol	Cheméo Relay (1.0)
hfus	36.09	kJ/mol	Joback Method
logp	4.855		Crippen Method
mcvol	212.460	ml/mol	McGowan Method
rinpol	2796.00		NIST Webbook
rinpol	2796.00		NIST Webbook
tb	701.18	K	Cheméo Relay (1.0)
tf	458.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.12	J/mol×K	840.86	Joback Method
cpg	570.25	J/mol×K	885.31	Joback Method
cpg	581.40	J/mol×K	929.76	Joback Method
cpg	591.75	J/mol×K	974.21	Joback Method
cpg	601.44	J/mol×K	1018.65	Joback Method
cpg	610.65	J/mol×K	1063.10	Joback Method
cpg	619.53	J/mol×K	1107.55	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C63295614&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

Cheméo Relay (1.0):

Legend

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

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