

Benzamide, n-(4-bromophenyl)-3-methyl-

Inchi:	InChI=1S/C14H12BrNO/c1-10-3-2-4-11(9-10)14(17)16-13-7-5-12(15)6-8-13/h2-9H,1H3,(
InchiKey:	WZXKTYYYMIAREML-UHFFFAOYSA-N
Formula:	C14H12BrNO
SMILES:	Cc1cccc(C(=O)Nc2ccc(Br)cc2)c1
Mol. weight [g/mol]:	290.16

Physical Properties

Property code	Value	Unit	Source
hf	-0.70	kJ/mol	Cheméo Relay (1.0)
hfus	31.30	kJ/mol	Joback Method
ie	8.06	eV	Cheméo Relay (1.0)
log10ws	-5.00		Cheméo Relay (1.0)
logp	4.010		Crippen Method
mcvol	189.650	ml/mol	McGowan Method
rinpol	2387.00		NIST Webbook
tb	644.48	K	Cheméo Relay (1.0)
tc	944.01	K	Cheméo Relay (1.0)
tf	421.55	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.27	J/mol×K	753.24	Joback Method
cpg	486.07	J/mol×K	795.83	Joback Method
cpg	497.75	J/mol×K	838.42	Joback Method
cpg	508.40	J/mol×K	881.01	Joback Method
cpg	518.11	J/mol×K	923.60	Joback Method
cpg	526.97	J/mol×K	966.19	Joback Method
cpg	535.06	J/mol×K	1008.78	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307116&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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