Benzamide, 4-bromo-N,N-diethyl-

Inchi: InChI=1S/C11H14BrNO/c1-3-13(4-2)11(14)9-5-7-10(12)8-6-9/h5-8H,3-4H2,1-2H3
InchiKey: LDUPVXSXLZOQAF-UHFFFAOYSA-N
Formula: C11H14BrNO
SMILES: CCN(CC)C(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 256.14

Physical Properties

Property code	Value	Unit	Source
gf	140.70	kJ/mol	Joback Method
hf	-64.03	kJ/mol	Joback Method
hfus	27.80	kJ/mol	Joback Method
hvap	58.24	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.931		Crippen Method
mcvol	171.140	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	1993.00		NIST Webbook
rinpol	1993.00		NIST Webbook
tb	615.21	K	Joback Method
tc	837.60	K	Joback Method
tf	394.87	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.83	J/mol×K	615.21	Joback Method
cpg	410.64	J/mol×K	652.27	Joback Method
cpg	423.49	J/mol×K	689.34	Joback Method
cpg	435.44	J/mol×K	726.40	Joback Method
cpg	446.56	J/mol×K	763.47	Joback Method
cpg	456.89	J/mol×K	800.53	Joback Method
cpg	466.49	J/mol×K	837.60	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415449&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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