

Benzamide, 2-bromo-N-ethyl-N-propyl-

Inchi:	InChI=1S/C12H16BrNO/c1-3-9-14(4-2)12(15)10-7-5-6-8-11(10)13/h5-8H,3-4,9H2,1-2H3
InchiKey:	BMRXZVFZTFOTLI-UHFFFAOYSA-N
Formula:	C12H16BrNO
SMILES:	CCCN(CC)C(=O)c1ccccc1Br
Mol. weight [g/mol]:	270.17

Physical Properties

Property code	Value	Unit	Source
gf	149.12	kJ/mol	Joback Method
hf	-84.67	kJ/mol	Joback Method
hfus	30.39	kJ/mol	Joback Method
hvap	60.47	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.321		Crippen Method
mcvol	185.230	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpola	2003.00		NIST Webbook
rinpola	2003.00		NIST Webbook
tb	638.09	K	Joback Method
tc	856.52	K	Joback Method
tf	406.14	K	Joback Method
vc	0.685	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.12	J/molxK	638.09	Joback Method
cpg	460.52	J/molxK	674.49	Joback Method
cpg	473.96	J/molxK	710.90	Joback Method
cpg	486.48	J/molxK	747.30	Joback Method
cpg	498.15	J/molxK	783.71	Joback Method
cpg	509.03	J/molxK	820.11	Joback Method
cpg	519.16	J/molxK	856.52	Joback Method

Sources

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=U415355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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