Benzamide, 2-bromo-N-ethyl-N-isobutyl-

Inchi: InChI=1S/C13H18BrNO/c1-4-15(9-10(2)3)13(16)11-7-5-6-8-12(11)14/h5-8,10H,4,9H2,1-3
InchiKey: HPLOSNOZXZYMLG-UHFFFAOYSA-N
Formula: C13H18BrNO
SMILES: CCN(CC(C)C)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 284.19

Physical Properties

Property code	Value	Unit	Source
gf	155.10	kJ/mol	Joback Method
hf	-110.59	kJ/mol	Joback Method
hfus	29.46	kJ/mol	Joback Method
hvap	62.31	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.567		Crippen Method
mcvol	199.320	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	660.53	K	Joback Method
tc	879.46	K	Joback Method
tf	402.41	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.34	J/mol×K	660.53	Joback Method
cpg	512.57	J/mol×K	697.02	Joback Method
cpg	526.78	J/mol×K	733.51	Joback Method
cpg	540.03	J/mol×K	769.99	Joback Method
cpg	552.36	J/mol×K	806.48	Joback Method
cpg	563.85	J/mol×K	842.97	Joback Method
cpg	574.56	J/mol×K	879.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U415356&Units=SI

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