Benzamide, 3-bromo-N-butyl-N-isobutyl-

Inchi: InChI=1S/C15H22BrNO/c1-4-5-9-17(11-12(2)3)15(18)13-7-6-8-14(16)10-13/h6-8,10,12H
InchiKey: VLPNMUNBRFBIGZ-UHFFFAOYSA-N
Formula: C15H22BrNO
SMILES: CCCCN(CC(C)C)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 312.25

Physical Properties

Property code	Value	Unit	Source
gf	171.94	kJ/mol	Joback Method
hf	-151.87	kJ/mol	Joback Method
hfus	34.64	kJ/mol	Joback Method
hvap	66.76	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.347		Crippen Method
mcvol	227.500	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook
tb	706.29	K	Joback Method
tc	918.43	K	Joback Method
tf	424.95	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.77	J/mol×K	706.29	Joback Method
cpg	618.78	J/mol×K	741.65	Joback Method
cpg	633.75	J/mol×K	777.00	Joback Method
cpg	647.76	J/mol×K	812.36	Joback Method
cpg	660.85	J/mol×K	847.72	Joback Method
cpg	673.09	J/mol×K	883.07	Joback Method
cpg	684.54	J/mol×K	918.43	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=U415659&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