Benzamide, 3-bromo-N-butyl-N-3-methylbutyl-

Inchi: InChI=1S/C16H24BrNO/c1-4-5-10-18(11-9-13(2)3)16(19)14-7-6-8-15(17)12-14/h6-8,12-1
InchiKey: OYBPTSWWAIRKJO-UHFFFAOYSA-N
Formula: C16H24BrNO
SMILES: CCCCN(CCC(C)C)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 326.27

Physical Properties

Property code	Value	Unit	Source
gf	180.36	kJ/mol	Joback Method
hf	-172.51	kJ/mol	Joback Method
hfus	37.23	kJ/mol	Joback Method
hvap	68.98	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.737		Crippen Method
mcvol	241.590	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2677.00		NIST Webbook
rinpol	2677.00		NIST Webbook
tb	729.17	K	Joback Method
tc	938.53	K	Joback Method
tf	436.22	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.30	J/mol×K	729.17	Joback Method
cpg	673.62	J/mol×K	764.06	Joback Method
cpg	688.90	J/mol×K	798.96	Joback Method
cpg	703.20	J/mol×K	833.85	Joback Method
cpg	716.60	J/mol×K	868.74	Joback Method
cpg	729.14	J/mol×K	903.64	Joback Method
cpg	740.90	J/mol×K	938.53	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=U415661&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