

Benzamide, 3-bromo-N-butyl-N-octyl-

Inchi:	InChI=1S/C19H30BrNO/c1-3-5-7-8-9-10-15-21(14-6-4-2)19(22)17-12-11-13-18(20)16-17
InchiKey:	MGZIFMARQOTNOH-UHFFFAOYSA-N
Formula:	C19H30BrNO
SMILES:	CCCCCCCCN(CCCC)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	368.35

Physical Properties

Property code	Value	Unit	Source
gf	208.06	kJ/mol	Joback Method
hf	-229.15	kJ/mol	Joback Method
hfus	48.52	kJ/mol	Joback Method
hvap	76.05	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	6.052		Crippen Method
mcvol	283.860	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	798.25	K	Joback Method
tc	999.82	K	Joback Method
tf	485.03	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.79	J/molxK	798.25	Joback Method
cpg	843.63	J/molxK	831.85	Joback Method
cpg	859.48	J/molxK	865.44	Joback Method
cpg	874.37	J/molxK	899.04	Joback Method
cpg	888.39	J/molxK	932.63	Joback Method
cpg	901.60	J/molxK	966.23	Joback Method
cpg	914.05	J/molxK	999.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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