Benzamide, 2-bromo-N-(2-bromobenzoyl)-N-butyl-

Inchi: InChI=1S/C18H17Br2NO2/c1-2-3-12-21(17(22)13-8-4-6-10-15(13)19)18(23)14-9-5-7-11-
InchiKey: IBDKYODHVYONML-UHFFFAOYSA-N
Formula: C18H17Br2NO2
SMILES: CCCCN(C(=O)c1ccccc1Br)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 439.14

Physical Properties

Property code	Value	Unit	Source
gf	187.82	kJ/mol	Joback Method
hf	-69.70	kJ/mol	Joback Method
hfus	46.47	kJ/mol	Joback Method
hvap	89.94	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	5.294		Crippen Method
mcvol	265.080	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	2708.00		NIST Webbook
rinpol	2708.00		NIST Webbook
tb	927.06	K	Joback Method
tc	1176.31	K	Joback Method
tf	622.43	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.27	J/mol×K	927.06	Joback Method
cpg	730.87	J/mol×K	968.60	Joback Method
cpg	741.59	J/mol×K	1010.14	Joback Method
cpg	751.56	J/mol×K	1051.68	Joback Method
cpg	760.90	J/mol×K	1093.23	Joback Method
cpg	769.74	J/mol×K	1134.77	Joback Method
cpg	778.21	J/mol×K	1176.31	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=U407068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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