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

Inchi: InChI=1S/C17H15Br2NO2/c1-2-11-20(16(21)12-7-3-5-9-14(12)18)17(22)13-8-4-6-10-15(

InchiKey: YBOHFNJJBGOLEY-UHFFFAOYSA-N

Formula: C17H15Br2NO2

SMILES: CCCN(C(=O)c1ccccc1Br)C(=O)c1ccccc1Br

Mol. weight [g/mol]: 425.12

Physical Properties

Property code	Value	Unit	Source
gf	179.40	kJ/mol	Joback Method
hf	-49.06	kJ/mol	Joback Method
hfus	43.88	kJ/mol	Joback Method
hvap	87.72	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	4.904		Crippen Method
mcvol	250.990	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	2621.00		NIST Webbook
rinpol	2621.00		NIST Webbook
tb	904.18	K	Joback Method
tc	1157.20	K	Joback Method
tf	611.16	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.15	J/mol×K	904.18	Joback Method
cpg	674.41	J/mol×K	946.35	Joback Method
cpg	684.77	J/mol×K	988.52	Joback Method
cpg	694.36	J/mol×K	1030.69	Joback Method
cpg	703.30	J/mol×K	1072.86	Joback Method
cpg	711.72	J/mol×K	1115.03	Joback Method
cpg	719.74	J/mol×K	1157.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407066&Units=SI
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

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