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

Inchi: InChI=1S/C19H19Br2NO2/c1-2-3-8-13-22(18(23)14-9-4-6-11-16(14)20)19(24)15-10-5-7-

InchiKey: PBJUOSSJIPUYDJ-UHFFFAOYSA-N

Formula: C19H19Br2NO2

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

Mol. weight [g/mol]: 453.17

Physical Properties

Property code	Value	Unit	Source
gf	196.24	kJ/mol	Joback Method
hf	-90.34	kJ/mol	Joback Method
hfus	49.06	kJ/mol	Joback Method
hvap	92.17	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	5.684		Crippen Method
mcvol	279.170	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	2813.00		NIST Webbook
rinpol	2813.00		NIST Webbook
tb	949.94	K	Joback Method
tc	1196.16	K	Joback Method
tf	633.70	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.22	J/mol×K	949.94	Joback Method
cpg	788.13	J/mol×K	990.98	Joback Method
cpg	799.19	J/mol×K	1032.01	Joback Method
cpg	809.53	J/mol×K	1073.05	Joback Method
cpg	819.26	J/mol×K	1114.09	Joback Method
cpg	828.52	J/mol×K	1155.13	Joback Method
cpg	837.42	J/mol×K	1196.16	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=U407070&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