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

Inchi: InChI=1S/C18H17Br2NO2/c1-12(2)11-21(17(22)13-7-3-5-9-15(13)19)18(23)14-8-4-6-10-

InchiKey: DUHNWGIQJIDONT-UHFFFAOYSA-N

Formula: C18H17Br2NO2

SMILES: CC(C)CN(C(=O)c1ccccc1Br)C(=O)c1ccccc1Br

Mol. weight [g/mol]: 439.14

Physical Properties

Property code	Value	Unit	Source
gf	185.38	kJ/mol	Joback Method
hf	-74.98	kJ/mol	Joback Method
hfus	42.95	kJ/mol	Joback Method
hvap	89.56	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.150		Crippen Method
mcvol	265.080	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	2665.00		NIST Webbook
rinpol	2665.00		NIST Webbook
tb	926.62	K	Joback Method
tc	1179.53	K	Joback Method
tf	607.43	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.80	J/mol×K	926.62	Joback Method
cpg	731.51	J/mol×K	968.77	Joback Method
cpg	742.30	J/mol×K	1010.92	Joback Method
cpg	752.30	J/mol×K	1053.08	Joback Method
cpg	761.64	J/mol×K	1095.23	Joback Method
cpg	770.46	J/mol×K	1137.38	Joback Method
cpg	778.89	J/mol×K	1179.53	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=U407067&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

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