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

Inchi: InChI=1S/C22H25Br2NO2/c1-3-5-10-16(4-2)15-25(21(26)17-11-6-8-13-19(17)23)22(27)1

InchiKey: HWMZHVJSKNSDJH-UHFFFAOYSA-N

Formula: C22H25Br2NO2

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

Mol. weight [g/mol]: 495.25

Physical Properties

Property code	Value	Unit	Source
gf	219.06	kJ/mol	Joback Method
hf	-157.54	kJ/mol	Joback Method
hfus	53.31	kJ/mol	Joback Method
hvap	98.46	kJ/mol	Joback Method
log10ws	-8.60		Crippen Method
logp	6.711		Crippen Method
mcvol	321.440	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	3005.00		NIST Webbook
rinpol	3005.00		NIST Webbook
tb	1018.14	K	Joback Method
tc	1262.28	K	Joback Method
tf	652.51	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.99	J/mol×K	1018.14	Joback Method
cpg	964.88	J/mol×K	1058.83	Joback Method
cpg	976.95	J/mol×K	1099.52	Joback Method
cpg	988.35	J/mol×K	1140.21	Joback Method
cpg	999.20	J/mol×K	1180.90	Joback Method
cpg	1009.65	J/mol×K	1221.59	Joback Method
cpg	1019.83	J/mol×K	1262.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407072&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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