Benzamide, 2-bromo-N-ethyl-N-pentyl-

Inchi: InChI=1S/C14H20BrNO/c1-3-5-8-11-16(4-2)14(17)12-9-6-7-10-13(12)15/h6-7,9-10H,3-5,
InchiKey: FQNDEBMOFIPTQX-UHFFFAOYSA-N
Formula: C14H20BrNO
SMILES: CCCCCN(CC)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 298.22

Physical Properties

Property code	Value	Unit	Source
gf	165.96	kJ/mol	Joback Method
hf	-125.95	kJ/mol	Joback Method
hfus	35.57	kJ/mol	Joback Method
hvap	64.92	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.101		Crippen Method
mcvol	213.410	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	2206.00		NIST Webbook
rinpol	2206.00		NIST Webbook
tb	683.85	K	Joback Method
tc	895.31	K	Joback Method
tf	428.68	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.91	J/mol×K	683.85	Joback Method
cpg	564.25	J/mol×K	719.09	Joback Method
cpg	578.61	J/mol×K	754.34	Joback Method
cpg	592.05	J/mol×K	789.58	Joback Method
cpg	604.61	J/mol×K	824.82	Joback Method
cpg	616.37	J/mol×K	860.07	Joback Method
cpg	627.37	J/mol×K	895.31	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=U415359&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