Benzamide, 2-bromo-N-ethyl-N-octyl-

Inchi: InChI=1S/C17H26BrNO/c1-3-5-6-7-8-11-14-19(4-2)17(20)15-12-9-10-13-16(15)18/h9-10
InchiKey: XKNXAFQWUBCYIH-UHFFFAOYSA-N
Formula: C17H26BrNO
SMILES: CCCCCCCCN(CC)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 340.30

Physical Properties

Property code	Value	Unit	Source
gf	191.22	kJ/mol	Joback Method
hf	-187.87	kJ/mol	Joback Method
hfus	43.34	kJ/mol	Joback Method
hvap	71.60	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.272		Crippen Method
mcvol	255.680	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2521.00		NIST Webbook
rinpol	2521.00		NIST Webbook
tb	752.49	K	Joback Method
tc	956.51	K	Joback Method
tf	462.49	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.42	J/mol×K	752.49	Joback Method
cpg	728.75	J/mol×K	786.49	Joback Method
cpg	744.08	J/mol×K	820.50	Joback Method
cpg	758.48	J/mol×K	854.50	Joback Method
cpg	772.00	J/mol×K	888.50	Joback Method
cpg	784.70	J/mol×K	922.51	Joback Method
cpg	796.65	J/mol×K	956.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415363&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