Benzamide, 2-bromo-N-ethyl-N-undecyl-

Inchi: InChI=1S/C20H32BrNO/c1-3-5-6-7-8-9-10-11-14-17-22(4-2)20(23)18-15-12-13-16-19(18
InchiKey: LYKIXGLNFITXIN-UHFFFAOYSA-N
Formula: C20H32BrNO
SMILES: CCCCCCCCCCCN(CC)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 382.38

Physical Properties

Property code	Value	Unit	Source
gf	216.48	kJ/mol	Joback Method
hf	-249.79	kJ/mol	Joback Method
hfus	51.11	kJ/mol	Joback Method
hvap	78.28	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	6.442		Crippen Method
mcvol	297.950	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	2945.00		NIST Webbook
rinpol	2945.00		NIST Webbook
tb	821.13	K	Joback Method
tc	1022.37	K	Joback Method
tf	496.30	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.38	J/mol×K	821.13	Joback Method
cpg	902.48	J/mol×K	854.67	Joback Method
cpg	918.56	J/mol×K	888.21	Joback Method
cpg	933.70	J/mol×K	921.75	Joback Method
cpg	947.96	J/mol×K	955.29	Joback Method
cpg	961.40	J/mol×K	988.83	Joback Method
cpg	974.08	J/mol×K	1022.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415366&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

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