Benzamide, N,N-dihexyl-3-bromo-

Inchi: InChI=1S/C19H30BrNO/c1-3-5-7-9-14-21(15-10-8-6-4-2)19(22)17-12-11-13-18(20)16-17
InchiKey: ZSIZDCDXEDUOSA-UHFFFAOYSA-N
Formula: C19H30BrNO
SMILES: CCCCCCN(CCCCCC)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 368.35

Physical Properties

Property code	Value	Unit	Source
gf	208.06	kJ/mol	Joback Method
hf	-229.15	kJ/mol	Joback Method
hfus	48.52	kJ/mol	Joback Method
hvap	76.05	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	6.052		Crippen Method
mcvol	283.860	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	2331.00		NIST Webbook
rinpol	2331.00		NIST Webbook
tb	798.25	K	Joback Method
tc	999.82	K	Joback Method
tf	485.03	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.79	J/mol×K	798.25	Joback Method
cpg	843.63	J/mol×K	831.85	Joback Method
cpg	859.48	J/mol×K	865.44	Joback Method
cpg	874.37	J/mol×K	899.04	Joback Method
cpg	888.39	J/mol×K	932.63	Joback Method
cpg	901.60	J/mol×K	966.23	Joback Method
cpg	914.05	J/mol×K	999.82	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=U308622&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