Benzamide, N-decyl-N-methyl-4-bromo-

Inchi: InChI=1S/C18H28BrNO/c1-3-4-5-6-7-8-9-10-15-20(2)18(21)16-11-13-17(19)14-12-16/h1
InchiKey: IVSUQHPPAYILPU-UHFFFAOYSA-N
Formula: C18H28BrNO
SMILES: CCCCCCCCCCN(C)C(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 354.32

Physical Properties

Property code	Value	Unit	Source
gf	199.64	kJ/mol	Joback Method
hf	-208.51	kJ/mol	Joback Method
hfus	45.93	kJ/mol	Joback Method
hvap	73.82	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.662		Crippen Method
mcvol	269.770	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	2490.00		NIST Webbook
tb	775.37	K	Joback Method
tc	977.89	K	Joback Method
tf	473.76	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.11	J/mol×K	775.37	Joback Method
cpg	785.71	J/mol×K	809.12	Joback Method
cpg	801.30	J/mol×K	842.88	Joback Method
cpg	815.96	J/mol×K	876.63	Joback Method
cpg	829.73	J/mol×K	910.38	Joback Method
cpg	842.69	J/mol×K	944.13	Joback Method
cpg	854.90	J/mol×K	977.89	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=U308454&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