Benzamide, 3-bromo-N-decyl-

Inchi: InChI=1S/C17H26BrNO/c1-2-3-4-5-6-7-8-9-13-19-17(20)15-11-10-12-16(18)14-15/h10-1
InchiKey: RBRUEJCZCYYUFR-UHFFFAOYSA-N
Formula: C17H26BrNO
SMILES: CCCCCCCCCCNC(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 340.30

Physical Properties

Property code	Value	Unit	Source
gf	169.83	kJ/mol	Joback Method
hf	-201.93	kJ/mol	Joback Method
hfus	45.42	kJ/mol	Joback Method
hvap	75.99	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.320		Crippen Method
mcvol	255.680	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tb	790.22	K	Joback Method
tc	997.20	K	Joback Method
tf	482.68	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.94	J/mol×K	790.22	Joback Method
cpg	744.49	J/mol×K	824.72	Joback Method
cpg	759.07	J/mol×K	859.21	Joback Method
cpg	772.75	J/mol×K	893.71	Joback Method
cpg	785.57	J/mol×K	928.21	Joback Method
cpg	797.61	J/mol×K	962.70	Joback Method
cpg	808.90	J/mol×K	997.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407213&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