Benzamide, 3-bromo-N-butyl-N-hept-2-yl-

Inchi: InChI=1S/C18H28BrNO/c1-4-6-8-10-15(3)20(13-7-5-2)18(21)16-11-9-12-17(19)14-16/h9
InchiKey: WGMKDCCHRKALCD-UHFFFAOYSA-N
Formula: C18H28BrNO
SMILES: CCCCCC(C)N(CCCC)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 354.32

Physical Properties

Property code	Value	Unit	Source
gf	197.20	kJ/mol	Joback Method
hf	-213.79	kJ/mol	Joback Method
hfus	42.41	kJ/mol	Joback Method
hvap	73.44	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.660		Crippen Method
mcvol	269.770	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	774.93	K	Joback Method
tc	980.19	K	Joback Method
tf	458.76	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.64	J/mol×K	774.93	Joback Method
cpg	786.46	J/mol×K	809.14	Joback Method
cpg	802.25	J/mol×K	843.35	Joback Method
cpg	817.06	J/mol×K	877.56	Joback Method
cpg	830.96	J/mol×K	911.77	Joback Method
cpg	844.01	J/mol×K	945.98	Joback Method
cpg	856.28	J/mol×K	980.19	Joback Method

Sources

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=U415663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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