Benzamide, 3-bromo-N-nonyl-

Inchi: InChI=1S/C16H24BrNO/c1-2-3-4-5-6-7-8-12-18-16(19)14-10-9-11-15(17)13-14/h9-11,13
InchiKey: KQJDMPZGMLJBGC-UHFFFAOYSA-N
Formula: C16H24BrNO
SMILES: CCCCCCCCCNC(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 326.27

Physical Properties

Property code	Value	Unit	Source
gf	161.41	kJ/mol	Joback Method
hf	-181.29	kJ/mol	Joback Method
hfus	42.83	kJ/mol	Joback Method
hvap	73.77	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	4.929		Crippen Method
mcvol	241.590	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	767.34	K	Joback Method
tc	976.03	K	Joback Method
tf	471.41	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.74	J/mol×K	767.34	Joback Method
cpg	687.98	J/mol×K	802.12	Joback Method
cpg	702.27	J/mol×K	836.90	Joback Method
cpg	715.67	J/mol×K	871.69	Joback Method
cpg	728.22	J/mol×K	906.47	Joback Method
cpg	739.98	J/mol×K	941.25	Joback Method
cpg	751.00	J/mol×K	976.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407212&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