Benzamide, 2-bromo-N-octyl-

Inchi: InChI=1S/C15H22BrNO/c1-2-3-4-5-6-9-12-17-15(18)13-10-7-8-11-14(13)16/h7-8,10-11H
InchiKey: YDGVXTKIJOPRSY-UHFFFAOYSA-N
Formula: C15H22BrNO
SMILES: CCCCCCCCNC(=O)c1ccccc1Br
Mol. weight [g/mol]: 312.25

Physical Properties

Property code	Value	Unit	Source
gf	152.99	kJ/mol	Joback Method
hf	-160.65	kJ/mol	Joback Method
hfus	40.24	kJ/mol	Joback Method
hvap	71.54	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.539		Crippen Method
mcvol	227.500	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	2328.00		NIST Webbook
rinpol	2328.00		NIST Webbook
tb	744.46	K	Joback Method
tc	955.40	K	Joback Method
tf	460.14	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.59	J/mol×K	744.46	Joback Method
cpg	632.50	J/mol×K	779.62	Joback Method
cpg	646.47	J/mol×K	814.77	Joback Method
cpg	659.55	J/mol×K	849.93	Joback Method
cpg	671.79	J/mol×K	885.09	Joback Method
cpg	683.25	J/mol×K	920.25	Joback Method
cpg	693.97	J/mol×K	955.40	Joback Method

Sources

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=U407119&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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