

Benzamide, 3-bromo-N-octyl-

Inchi:	InChI=1S/C15H22BrNO/c1-2-3-4-5-6-7-11-17-15(18)13-9-8-10-14(16)12-13/h8-10,12H,2
InchiKey:	DRVXITPEDPBBSZ-UHFFFAOYSA-N
Formula:	C15H22BrNO
SMILES:	CCCCCCCCNC(=O)c1cccc(Br)c1
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
mvol	227.500	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	2379.00		NIST Webbook
rinpol	2379.00		NIST Webbook
tb	744.46	K	Joback Method
tc	955.40	K	Joback Method
tf	460.14	K	Joback Method
vc	0.871	m ³ /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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407211&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
h vap:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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