Benzamide, N-tetrahydrofurfuryl-2-bromo-

Inchi: InChI=1S/C12H14BrNO2/c13-11-6-2-1-5-10(11)12(15)14-8-9-4-3-7-16-9/h1-2,5-6,9H,3-4
InchiKey: AMXQJNHGAOPECX-UHFFFAOYSA-N
Formula: C12H14BrNO2
SMILES: O=C(NCC1CCCO1)c1ccccc1Br
Mol. weight [g/mol]: 284.15

Physical Properties

Property code	Value	Unit	Source
gf	78.16	kJ/mol	Joback Method
hf	-170.25	kJ/mol	Joback Method
hfus	34.38	kJ/mol	Joback Method
hvap	69.63	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.358		Crippen Method
mcvol	180.240	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	2063.00		NIST Webbook
rinpol	2063.00		NIST Webbook
tb	718.05	K	Joback Method
tc	964.82	K	Joback Method
tf	463.80	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.86	J/mol×K	718.05	Joback Method
cpg	491.34	J/mol×K	759.18	Joback Method
cpg	504.61	J/mol×K	800.31	Joback Method
cpg	516.77	J/mol×K	841.44	Joback Method
cpg	527.88	J/mol×K	882.57	Joback Method
cpg	538.05	J/mol×K	923.69	Joback Method
cpg	547.34	J/mol×K	964.82	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=U307383&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