Benzamide, N-(4-fluorophenyl)-3-bromo-

Inchi: InChI=1S/C13H9BrFNO/c14-10-3-1-2-9(8-10)13(17)16-12-6-4-11(15)5-7-12/h1-8H,(H,16
InchiKey: RALCKMXGUGIREZ-UHFFFAOYSA-N
Formula: C13H9BrFNO
SMILES: O=C(Nc1ccc(F)cc1)c1cccc(Br)c1
Mol. weight [g/mol]: 294.12

Physical Properties

Property code	Value	Unit	Source
gf	44.12	kJ/mol	Joback Method
hf	-90.42	kJ/mol	Joback Method
hfus	31.79	kJ/mol	Joback Method
hvap	69.21	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.840		Crippen Method
mcvol	177.330	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	2198.00		NIST Webbook
rinpol	2198.00		NIST Webbook
tb	729.63	K	Joback Method
tc	979.25	K	Joback Method
tf	477.13	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.72	J/mol×K	729.63	Joback Method
cpg	441.35	J/mol×K	771.23	Joback Method
cpg	451.94	J/mol×K	812.84	Joback Method
cpg	461.58	J/mol×K	854.44	Joback Method
cpg	470.34	J/mol×K	896.04	Joback Method
cpg	478.31	J/mol×K	937.65	Joback Method
cpg	485.56	J/mol×K	979.25	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=U307152&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