Benzamide, 2,3,4-trifluoro-N-(2-bromophenyl)-

Inchi: InChI=1S/C13H7BrF3NO/c14-8-3-1-2-4-10(8)18-13(19)7-5-6-9(15)12(17)11(7)16/h1-6H,(
InchiKey: GEMNMIUWKPRTOY-UHFFFAOYSA-N
Formula: C13H7BrF3NO
SMILES: O=C(Nc1ccccc1Br)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 330.10

Physical Properties

Property code	Value	Unit	Source
gf	-364.76	kJ/mol	Joback Method
hf	-505.58	kJ/mol	Joback Method
hfus	37.18	kJ/mol	Joback Method
hvap	68.90	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.119		Crippen Method
mcvol	180.870	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
tb	738.13	K	Joback Method
tc	968.25	K	Joback Method
tf	503.35	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.21	J/mol×K	738.13	Joback Method
cpg	452.44	J/mol×K	776.48	Joback Method
cpg	461.84	J/mol×K	814.84	Joback Method
cpg	470.44	J/mol×K	853.19	Joback Method
cpg	478.31	J/mol×K	891.55	Joback Method
cpg	485.49	J/mol×K	929.90	Joback Method
cpg	492.03	J/mol×K	968.25	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=U340220&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