Acetamide, N-(4-bromophenyl)-2,2,2-trifluoro-

Inchi: InChI=1S/C8H5BrF3NO/c9-5-1-3-6(4-2-5)13-7(14)8(10,11)12/h1-4H,(H,13,14)
InchiKey: VVFVNAMWSGDFCX-UHFFFAOYSA-N
Formula: C8H5BrF3NO
SMILES: O=C(Nc1ccc(Br)cc1)C(F)(F)F
Mol. weight [g/mol]: 268.03

Physical Properties

Property code	Value	Unit	Source
gf	-487.54	kJ/mol	Joback Method
hf	-613.25	kJ/mol	Joback Method
hfus	23.94	kJ/mol	Joback Method
hvap	52.21	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.950		Crippen Method
mcvol	134.180	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
rinpol	1376.00		NIST Webbook
rinpol	1376.00		NIST Webbook
tb	578.88	K	Joback Method
tc	796.67	K	Joback Method
tf	385.44	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.17	J/mol×K	578.88	Joback Method
cpg	305.72	J/mol×K	615.18	Joback Method
cpg	314.45	J/mol×K	651.48	Joback Method
cpg	322.42	J/mol×K	687.77	Joback Method
cpg	329.68	J/mol×K	724.07	Joback Method
cpg	336.30	J/mol×K	760.37	Joback Method
cpg	342.33	J/mol×K	796.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307312&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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