Acetamide, N-(4-fluorophenyl)-2-bromo-

Inchi: InChI=1S/C8H7BrFNO/c9-5-8(12)11-7-3-1-6(10)2-4-7/h1-4H,5H2,(H,11,12)
InchiKey: JXUWYCOGYOQUST-UHFFFAOYSA-N
Formula: C8H7BrFNO
SMILES: O=C(CBr)Nc1ccc(F)cc1
Mol. weight [g/mol]: 232.05

Physical Properties

Property code	Value	Unit	Source
gf	-100.76	kJ/mol	Joback Method
hf	-212.28	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	55.14	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.159		Crippen Method
mcvol	130.640	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
rinpol	1525.00		NIST Webbook
tb	583.57	K	Joback Method
tc	809.93	K	Joback Method
tf	381.84	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.72	J/mol×K	583.57	Joback Method
cpg	285.77	J/mol×K	621.30	Joback Method
cpg	295.08	J/mol×K	659.02	Joback Method
cpg	303.69	J/mol×K	696.75	Joback Method
cpg	311.64	J/mol×K	734.48	Joback Method
cpg	318.99	J/mol×K	772.20	Joback Method
cpg	325.75	J/mol×K	809.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307418&Units=SI

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