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

Inchi: InChI=1S/C9H9BrFNO/c1-6(10)9(13)12-8-4-2-7(11)3-5-8/h2-6H,1H3,(H,12,13)
InchiKey: ZYPHUTLRFAVKHO-UHFFFAOYSA-N
Formula: C9H9BrFNO
SMILES: CC(Br)C(=O)Nc1ccc(F)cc1
Mol. weight [g/mol]: 246.08

Physical Properties

Property code	Value	Unit	Source
gf	-94.78	kJ/mol	Joback Method
hf	-238.20	kJ/mol	Joback Method
hfus	24.26	kJ/mol	Joback Method
hvap	56.98	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.548		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinpol	1537.00		NIST Webbook
tb	606.01	K	Joback Method
tc	832.91	K	Joback Method
tf	378.11	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.74	J/mol×K	606.01	Joback Method
cpg	332.96	J/mol×K	643.83	Joback Method
cpg	343.37	J/mol×K	681.64	Joback Method
cpg	353.00	J/mol×K	719.46	Joback Method
cpg	361.90	J/mol×K	757.27	Joback Method
cpg	370.12	J/mol×K	795.09	Joback Method
cpg	377.70	J/mol×K	832.91	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=U307474&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