3-Fluoro-5-trifluoromethylbenzamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C14H8BrF4NO/c15-10-1-3-12(4-2-10)20-13(21)8-5-9(14(17,18)19)7-11(16)6-8

InchiKey: SOPFRYSXMODMRA-UHFFFAOYSA-N

Formula: C14H8BrF4NO

SMILES: O=C(Nc1ccc(Br)cc1)c1cc(F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 362.12

Physical Properties

Property code	Value	Unit	Source
gf	-538.68	kJ/mol	Joback Method
hf	-719.61	kJ/mol	Joback Method
hfus	35.82	kJ/mol	Joback Method
hvap	68.35	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.859		Crippen Method
mcvol	196.730	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	2210.00		NIST Webbook
tb	752.07	K	Joback Method
tc	979.70	K	Joback Method
tf	505.11	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.60	J/mol×K	752.07	Joback Method
cpg	516.12	J/mol×K	790.01	Joback Method
cpg	525.73	J/mol×K	827.95	Joback Method
cpg	534.51	J/mol×K	865.88	Joback Method
cpg	542.54	J/mol×K	903.82	Joback Method
cpg	549.92	J/mol×K	941.76	Joback Method
cpg	556.72	J/mol×K	979.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358151&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