2,6-Difluoro-3-methylbenzamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C14H10BrF2NO/c1-8-2-7-11(16)12(13(8)17)14(19)18-10-5-3-9(15)4-6-10/h2-7

InchiKey: PDDRMXCGVINYRF-UHFFFAOYSA-N

Formula: C14H10BrF2NO

SMILES: Cc1ccc(F)c(C(=O)Nc2ccc(Br)cc2)c1F

Mol. weight [g/mol]: 326.14

Physical Properties

Property code	Value	Unit	Source
gf	-161.53	kJ/mol	Joback Method
hf	-330.11	kJ/mol	Joback Method
hfus	36.68	kJ/mol	Joback Method
hvap	71.94	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.288		Crippen Method
mcvol	193.190	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	2419.00		NIST Webbook
tb	761.74	K	Joback Method
tc	997.40	K	Joback Method
tf	514.03	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.74	J/mol×K	761.74	Joback Method
cpg	497.06	J/mol×K	801.02	Joback Method
cpg	507.47	J/mol×K	840.29	Joback Method
cpg	517.02	J/mol×K	879.57	Joback Method
cpg	525.76	J/mol×K	918.85	Joback Method
cpg	533.75	J/mol×K	958.13	Joback Method
cpg	541.05	J/mol×K	997.40	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=U358107&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