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

Inchi: InChI=1S/C14H10F3NO/c1-8-2-7-11(16)12(13(8)17)14(19)18-10-5-3-9(15)4-6-10/h2-7H,

InchiKey: OPKAAOMTPXRTOR-UHFFFAOYSA-N

Formula: C14H10F3NO

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

Mol. weight [g/mol]: 265.23

Physical Properties

Property code	Value	Unit	Source
gf	-370.66	kJ/mol	Joback Method
hf	-552.55	kJ/mol	Joback Method
hfus	34.48	kJ/mol	Joback Method
hvap	64.69	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.665		Crippen Method
mcvol	177.460	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		NIST Webbook
tb	694.85	K	Joback Method
tc	911.04	K	Joback Method
tf	454.82	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.73	J/mol×K	694.85	Joback Method
cpg	473.02	J/mol×K	730.88	Joback Method
cpg	484.43	J/mol×K	766.91	Joback Method
cpg	495.00	J/mol×K	802.94	Joback Method
cpg	504.77	J/mol×K	838.97	Joback Method
cpg	513.76	J/mol×K	875.00	Joback Method
cpg	522.03	J/mol×K	911.04	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=U358102&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