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

Inchi: InChI=1S/C15H13F2NO2/c1-9-3-8-12(16)13(14(9)17)15(19)18-10-4-6-11(20-2)7-5-10/h3

InchiKey: QBISXJFNWXVIRJ-UHFFFAOYSA-N

Formula: C15H13F2NO2

SMILES: COc1ccc(NC(=O)c2c(F)ccc(C)c2F)cc1

Mol. weight [g/mol]: 277.27

Physical Properties

Property code	Value	Unit	Source
gf	-272.43	kJ/mol	Joback Method
hf	-509.30	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	70.14	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.534		Crippen Method
mcvol	195.650	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	2369.00		NIST Webbook
rinpol	2369.00		NIST Webbook
tb	740.88	K	Joback Method
tc	960.28	K	Joback Method
tf	487.73	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.95	J/mol×K	740.88	Joback Method
cpg	543.00	J/mol×K	777.45	Joback Method
cpg	555.09	J/mol×K	814.01	Joback Method
cpg	566.25	J/mol×K	850.58	Joback Method
cpg	576.48	J/mol×K	887.15	Joback Method
cpg	585.82	J/mol×K	923.72	Joback Method
cpg	594.29	J/mol×K	960.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358105&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

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