2,6-Difluoro-3-methylbenzamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C15H13F2NO/c1-9-4-3-5-11(8-9)18-15(19)13-12(16)7-6-10(2)14(13)17/h3-8H,

InchiKey: KSYNOUFKEDSJDO-UHFFFAOYSA-N

Formula: C15H13F2NO

SMILES: Cc1cccc(NC(=O)c2c(F)ccc(C)c2F)c1

Mol. weight [g/mol]: 261.27

Physical Properties

Property code	Value	Unit	Source
gf	-167.43	kJ/mol	Joback Method
hf	-377.08	kJ/mol	Joback Method
hfus	33.99	kJ/mol	Joback Method
hvap	67.73	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.834		Crippen Method
mcvol	189.780	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
tb	718.46	K	Joback Method
tc	940.28	K	Joback Method
tf	465.50	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.39	J/mol×K	718.46	Joback Method
cpg	517.78	J/mol×K	755.43	Joback Method
cpg	530.21	J/mol×K	792.40	Joback Method
cpg	541.72	J/mol×K	829.37	Joback Method
cpg	552.34	J/mol×K	866.34	Joback Method
cpg	562.13	J/mol×K	903.31	Joback Method
cpg	571.11	J/mol×K	940.28	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=U358103&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