2,4,5-Trifluoro-3-methoxybenzamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C15H12F3NO2/c1-8-4-3-5-9(6-8)19-15(20)10-7-11(16)13(18)14(21-2)12(10)17

InchiKey: GPYGTFIAMRVYEE-UHFFFAOYSA-N

Formula: C15H12F3NO2

SMILES: COc1c(F)c(F)cc(C(=O)Nc2cccc(C)c2)c1F

Mol. weight [g/mol]: 295.26

Physical Properties

Property code	Value	Unit	Source
gf	-476.87	kJ/mol	Joback Method
hf	-716.88	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	69.99	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	3.673		Crippen Method
mcvol	197.420	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	2192.00		NIST Webbook
tb	745.13	K	Joback Method
tc	957.08	K	Joback Method
tf	500.84	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.49	J/mol×K	745.13	Joback Method
cpg	548.86	J/mol×K	780.45	Joback Method
cpg	560.35	J/mol×K	815.78	Joback Method
cpg	570.97	J/mol×K	851.10	Joback Method
cpg	580.74	J/mol×K	886.43	Joback Method
cpg	589.68	J/mol×K	921.75	Joback Method
cpg	597.79	J/mol×K	957.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358066&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