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

Inchi: InChI=1S/C15H12F3NO3/c1-21-9-5-3-8(4-6-9)19-15(20)10-7-11(16)13(18)14(22-2)12(10
InchiKey: AEVAKSCYZBAMQQ-UHFFFAOYSA-N
Formula: C15H12F3NO3
SMILES: COc1ccc(NC(=O)c2cc(F)c(F)c(OC)c2F)cc1
Mol. weight [g/mol]: 311.26

Physical Properties

Property code	Value	Unit	Source
gf	-581.87	kJ/mol	Joback Method
hf	-849.10	kJ/mol	Joback Method
hfus	39.06	kJ/mol	Joback Method
hvap	72.40	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.373		Crippen Method
mcvol	203.290	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	2374.00		NIST Webbook
rinpol	2374.00		NIST Webbook
tb	767.55	K	Joback Method
tc	977.97	K	Joback Method
tf	523.07	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.05	J/mol×K	767.55	Joback Method
cpg	574.12	J/mol×K	802.62	Joback Method
cpg	585.28	J/mol×K	837.69	Joback Method
cpg	595.52	J/mol×K	872.76	Joback Method
cpg	604.86	J/mol×K	907.83	Joback Method
cpg	613.29	J/mol×K	942.90	Joback Method
cpg	620.80	J/mol×K	977.97	Joback Method

Sources

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=U358068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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