4-Methoxybenzene-1,3-diamine, N1,N1,N3,N3-tetrakis(trifluoroacetyl)-

Inchi: InChI=1S/C15H6F12N2O5/c1-34-7-3-2-5(28(8(30)12(16,17)18)9(31)13(19,20)21)4-6(7)2

InchiKey: FFLAXRAEONXGQI-UHFFFAOYSA-N

Formula: C15H6F12N2O5

SMILES: COc1ccc(N(C(=O)C(F)(F)F)C(=O)C(F)(F)F)cc1N(C(=O)C(F)(F)F)C(=O)C(F)(F)F

Mol. weight [g/mol]: 522.20

Physical Properties

Property code	Value	Unit	Source
gf	-2556.91	kJ/mol	Joback Method
hf	-2975.14	kJ/mol	Joback Method
hfus	48.80	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.664		Crippen Method
mcvol	251.800	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	1376.00		NIST Webbook
tb	820.34	K	Joback Method
tc	1006.13	K	Joback Method
tf	613.92	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.58	J/mol×K	820.34	Joback Method
cpg	779.70	J/mol×K	851.31	Joback Method
cpg	787.07	J/mol×K	882.27	Joback Method
cpg	793.80	J/mol×K	913.24	Joback Method
cpg	799.97	J/mol×K	944.20	Joback Method
cpg	805.66	J/mol×K	975.17	Joback Method
cpg	810.96	J/mol×K	1006.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373466&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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