4-Methoxybenzene-1,3-diamine, N1,N3-bis(trifluorocetyl)-

Inchi: InChI=1S/C11H8F6N2O3/c1-22-7-3-2-5(18-8(20)10(12,13)14)4-6(7)19-9(21)11(15,16)17

InchiKey: ZAYHFAFCYKRUFT-UHFFFAOYSA-N

Formula: C11H8F6N2O3

SMILES: COc1ccc(NC(=O)C(F)(F)F)cc1NC(=O)C(F)(F)F

Mol. weight [g/mol]: 330.18

Physical Properties

Property code	Value	Unit	Source
gf	-1212.35	kJ/mol	Joback Method
hf	-1501.38	kJ/mol	Joback Method
hfus	35.74	kJ/mol	Joback Method
hvap	64.96	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.697		Crippen Method
mcvol	181.680	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1688.00		NIST Webbook
tb	707.38	K	Joback Method
tc	897.45	K	Joback Method
tf	500.98	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.05	J/mol×K	707.38	Joback Method
cpg	522.73	J/mol×K	739.06	Joback Method
cpg	531.67	J/mol×K	770.74	Joback Method
cpg	539.90	J/mol×K	802.41	Joback Method
cpg	547.46	J/mol×K	834.09	Joback Method
cpg	554.41	J/mol×K	865.77	Joback Method
cpg	560.77	J/mol×K	897.45	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373210&Units=SI

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