2-Methylbenzene-1,4-diamine, tris(trifluoroacetyl)-, isomer 1

Other names: 2,2-Bis-trifluoroacetamino-5-trifluoroacetamino-toluene
Inchi: InChI=1S/C13H7F9N2O3/c1-5-4-6(23-8(25)11(14,15)16)2-3-7(5)24(9(26)12(17,18)19)10
InchiKey: PLJMMVVKQYYODO-UHFFFAOYSA-N
Formula: C13H7F9N2O3
SMILES: Cc1cc(NC(=O)C(F)(F)F)ccc1N(C(=O)C(F)(F)F)C(=O)C(F)(F)F
Mol. weight [g/mol]: 410.19

Physical Properties

Property code	Value	Unit	Source
gf	-1779.63	kJ/mol	Joback Method
hf	-2106.04	kJ/mol	Joback Method
hfus	41.08	kJ/mol	Joback Method
hvap	65.61	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.480		Crippen Method
mcvol	210.870	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	1399.00		NIST Webbook
rinpol	1399.00		NIST Webbook
tb	741.44	K	Joback Method
tc	924.16	K	Joback Method
tf	535.22	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.90	J/mol×K	741.44	Joback Method
cpg	626.95	J/mol×K	771.89	Joback Method
cpg	635.25	J/mol×K	802.35	Joback Method
cpg	642.85	J/mol×K	832.80	Joback Method
cpg	649.84	J/mol×K	863.25	Joback Method
cpg	656.28	J/mol×K	893.71	Joback Method
cpg	662.24	J/mol×K	924.16	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=U378211&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