1,2-Phenylenediamine, N,N'-bis(trifluoroacetyl)-

Inchi: InChI=1S/C10H6F6N2O2/c11-9(12,13)7(19)17-5-3-1-2-4-6(5)18-8(20)10(14,15)16/h1-4H

InchiKey: FPBBQCMIENMBEO-UHFFFAOYSA-N

Formula: C10H6F6N2O2

SMILES: O=C(Nc1ccccc1NC(=O)C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 300.16

Physical Properties

Property code	Value	Unit	Source
hf	-1479.79	kJ/mol	Cheméo Relay (1.0)
hfus	32.36	kJ/mol	Joback Method
ie	8.86	eV	Cheméo Relay (1.0)
log10ws	-3.13		Cheméo Relay (1.0)
logp	2.688		Crippen Method
mcvol	161.720	ml/mol	McGowan Method
rinpol	1418.00		NIST Webbook
tb	505.21	K	Cheméo Relay (1.0)
tf	422.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.19	J/mol×K	657.10	Joback Method
cpg	450.74	J/mol×K	689.02	Joback Method
cpg	459.50	J/mol×K	720.94	Joback Method
cpg	467.52	J/mol×K	752.85	Joback Method
cpg	474.85	J/mol×K	784.77	Joback Method
cpg	481.57	J/mol×K	816.69	Joback Method
cpg	487.71	J/mol×K	848.61	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14818623&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point