N-(2,2,3,3,3-Pentafluoropropanoyl)-N-(4-((2,2,3,3,3

Other names: Benzene-1,4-diamine, tris(pentafuoropropionate)
Inchi: InChI=1S/C15H5F15N2O3/c16-10(17,13(22,23)24)7(33)31-5-1-3-6(4-2-5)32(8(34)11(18,
InchiKey: RTYRCGYEMCAEBA-UHFFFAOYSA-N
Formula: C15H5F15N2O3
SMILES: O=C(Nc1ccc(N(C(=O)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)F)cc1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 546.19

Physical Properties

Property code	Value	Unit	Source
gf	-2913.50	kJ/mol	Joback Method
hf	-3338.76	kJ/mol	Joback Method
hfus	42.89	kJ/mol	Joback Method
hvap	60.61	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.077		Crippen Method
mcvol	249.670	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1386.00		NIST Webbook
tb	768.15	K	Joback Method
tc	943.80	K	Joback Method
tf	556.04	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.95	J/mol×K	768.15	Joback Method
cpg	786.30	J/mol×K	797.43	Joback Method
cpg	793.87	J/mol×K	826.70	Joback Method
cpg	800.76	J/mol×K	855.98	Joback Method
cpg	807.09	J/mol×K	885.25	Joback Method
cpg	812.97	J/mol×K	914.53	Joback Method
cpg	818.48	J/mol×K	943.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373240&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

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