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

Inchi: InChI=1S/C16H7F15N2O3/c1-5-4-6(32-8(34)11(17,18)14(23,24)25)2-3-7(5)33(9(35)12(1

InchiKey: ICGBRHKCSSATGU-UHFFFAOYSA-N

Formula: C16H7F15N2O3

SMILES: Cc1cc(NC(=O)C(F)(F)C(F)(F)F)ccc1N(C(=O)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 560.21

Physical Properties

Property code	Value	Unit	Source
gf	-2914.71	kJ/mol	Joback Method
hf	-3370.87	kJ/mol	Joback Method
hfus	45.09	kJ/mol	Joback Method
hvap	63.50	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.386		Crippen Method
mcvol	263.760	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	1376.00		NIST Webbook
tb	796.01	K	Joback Method
tc	975.90	K	Joback Method
tf	579.83	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.03	J/mol×K	796.01	Joback Method
cpg	837.72	J/mol×K	825.99	Joback Method
cpg	845.67	J/mol×K	855.97	Joback Method
cpg	852.98	J/mol×K	885.96	Joback Method
cpg	859.78	J/mol×K	915.94	Joback Method
cpg	866.17	J/mol×K	945.92	Joback Method
cpg	872.26	J/mol×K	975.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378213&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