

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

Inchi: InChI=1S/C19H7F21N2O3/c1-5-4-6(2-3-7(5)41-8(43)11(20,21)14(26,27)17(32,33)34)42(35,36)37(38,39)31(40,41)30(42,43)29(44,45)28(46,47)27(48,49)26(50,51)25(52,53)24(54,55)23(56,57)22(58,59)21(60,61)20(62,63)19(64,65)18(66,67)16(68,69)15(70,71)13(72,73)12(74,75)10(76,77)9(78,79)8(80,81)7(82,83)6(84,85)5(86,87)4(88,89)3(90,91)2(92,93)1(94,95)H/t1-19/m1-19/s1-19/b1-19

InchiKey: GICPJXNHQDQJPA-UHFFFAOYSA-N

Formula: C19H7F21N2O3

SMILES: Cc1cc(N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)C(F)(F)F)ccc1NC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 710.24

Physical Properties

Property code	Value	Unit	Source
gf	-4049.79	kJ/mol	Joback Method
hf	-4635.70	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	61.38	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	7.292		Crippen Method
mcvol	316.650	ml/mol	McGowan Method
pc	909.98	kPa	Joback Method
rinpol	1484.00		NIST Webbook
rinpol	1484.00		NIST Webbook
tb	850.58	K	Joback Method
tc	1044.93	K	Joback Method
tf	624.44	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.57	J/mol×K	850.58	Joback Method
cpg	1050.49	J/mol×K	882.97	Joback Method
cpg	1058.74	J/mol×K	915.36	Joback Method
cpg	1066.53	J/mol×K	947.75	Joback Method
cpg	1074.06	J/mol×K	980.15	Joback Method
cpg	1081.51	J/mol×K	1012.54	Joback Method
cpg	1089.09	J/mol×K	1044.93	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=U378210&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
hvac:	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

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