

2-Methylbenzene-1,4-diamine, N1,N4-bis(pentafluoropropionyl)-

Other names:	2,5-Bis(pentafluoropropionylamino)toluene
Inchi:	InChI=1S/C13H8F10N2O2/c1-5-4-6(24-8(26)10(14,15)12(18,19)20)2-3-7(5)25-9(27)11(1
InchiKey:	KIEUVGHKDXZHCS-UHFFFAOYSA-N
Formula:	C13H8F10N2O2
SMILES:	Cc1cc(NC(=O)C(F)(F)C(F)(F)F)ccc1NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	414.20

Physical Properties

Property code	Value	Unit	Source
gf	-1864.07	kJ/mol	Joback Method
hf	-2212.38	kJ/mol	Joback Method
hfus	37.23	kJ/mol	Joback Method
hvap	61.14	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.267		Crippen Method
mcvol	211.070	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	1574.00		NIST Webbook
rinpol	1574.00		NIST Webbook
tb	721.34	K	Joback Method
tc	901.23	K	Joback Method
tf	508.49	K	Joback Method
vc	0.874	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.29	J/mol×K	721.34	Joback Method
cpg	637.87	J/mol×K	751.32	Joback Method
cpg	646.66	J/mol×K	781.30	Joback Method
cpg	654.73	J/mol×K	811.28	Joback Method
cpg	662.16	J/mol×K	841.27	Joback Method
cpg	669.01	J/mol×K	871.25	Joback Method
cpg	675.38	J/mol×K	901.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U373218&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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