

2-Methylbenzene-1,4-diamine, N1,N1,N4,N4-tetrakis(trifluoroacetyl)--

Other names:	2,5-Bis-di-trifluoroacetaminotoluene
Inchi:	InChI=1S/C15H6F12N2O4/c1-5-4-6(28(8(30)12(16,17)18)9(31)13(19,20)21)2-3-7(5)29(1
InchiKey:	ZJPZWBQEOFWYOT-UHFFFAOYSA-N
Formula:	C15H6F12N2O4
SMILES:	<chem>Cc1cc(N(C(=O)C(F)(F)F)C(=O)C(F)(F)F)ccc1N(C(=O)C(F)(F)F)C(=O)C(F)(F)F</chem>
Mol. weight [g/mol]:	506.20

Physical Properties

Property code	Value	Unit	Source
gf	-2451.91	kJ/mol	Joback Method
hf	-2842.92	kJ/mol	Joback Method
hfus	47.61	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.963		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	1236.00		NIST Webbook
tb	797.92	K	Joback Method
tc	980.52	K	Joback Method
tf	591.69	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.30	J/molxK	797.92	Joback Method
cpg	755.59	J/molxK	828.35	Joback Method
cpg	763.16	J/molxK	858.79	Joback Method
cpg	770.10	J/molxK	889.22	Joback Method
cpg	776.49	J/molxK	919.65	Joback Method
cpg	782.43	J/molxK	950.09	Joback Method
cpg	788.02	J/molxK	980.52	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=U373467&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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