

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

Other names:	2,5-Bis(heptafluorobutyrylamino)toluene
Inchi:	InChI=1S/C15H8F14N2O2/c1-5-4-6(30-8(32)10(16,17)12(20,21)14(24,25)26)2-3-7(5)31-
InchiKey:	CKNOZWDPTIZQOH-UHFFFAOYSA-N
Formula:	C15H8F14N2O2
SMILES:	<chem>Cc1cc(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)ccc1NC(=O)C(F)(F)C(F)(F)C(F)(F)F</chem>
Mol. weight [g/mol]:	514.21

Physical Properties

Property code	Value	Unit	Source
gf	-2620.79	kJ/mol	Joback Method
hf	-3055.60	kJ/mol	Joback Method
hfus	39.90	kJ/mol	Joback Method
hvap	59.73	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	5.538		Crippen Method
mcvol	246.330	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	1638.00		NIST Webbook
tb	757.72	K	Joback Method
tc	933.31	K	Joback Method
tf	538.23	K	Joback Method
vc	1.036	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.04	J/molxK	757.72	Joback Method
cpg	778.31	J/molxK	786.98	Joback Method
cpg	786.79	J/molxK	816.25	Joback Method
cpg	794.58	J/molxK	845.51	Joback Method
cpg	801.78	J/molxK	874.78	Joback Method
cpg	808.48	J/molxK	904.04	Joback Method
cpg	814.78	J/molxK	933.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U373220&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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