N-(2,2,3,3,4,4,4-Heptafluorobutanoyl)-N-(4-((2,2,3,3

Other names: Benzene-1,4-diamine, tris(heptafluorobutyrate)
Inchi: InChI=1S/C18H5F21N2O3/c19-10(20,13(25,26)16(31,32)33)7(42)40-5-1-3-6(4-2-5)41(8(
InchiKey: VBZSUDZUWCNOIS-UHFFFAOYSA-N
Formula: C18H5F21N2O3
SMILES: O=C(Nc1ccc(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)cc1)C(F)(F)
Mol. weight [g/mol]: 696.21

Physical Properties

Property code	Value	Unit	Source
gf	-4048.58	kJ/mol	Joback Method
hf	-4603.59	kJ/mol	Joback Method
hfus	46.90	kJ/mol	Joback Method
hvap	58.50	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	6.983		Crippen Method
mcvol	302.560	ml/mol	McGowan Method
pc	974.13	kPa	Joback Method
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
tb	822.72	K	Joback Method
tc	1008.56	K	Joback Method
tf	600.65	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.28	J/mol×K	822.72	Joback Method
cpg	997.62	J/mol×K	853.69	Joback Method
cpg	1005.23	J/mol×K	884.67	Joback Method
cpg	1012.28	J/mol×K	915.64	Joback Method
cpg	1018.95	J/mol×K	946.61	Joback Method
cpg	1025.42	J/mol×K	977.59	Joback Method
cpg	1031.86	J/mol×K	1008.56	Joback Method

Sources

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=U373241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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