1,4-Bis(heptafluoroisopropyl)benzene

Inchi: InChI=1S/C12H4F14/c13-7(9(15,16)17,10(18,19)20)5-1-2-6(4-3-5)8(14,11(21,22)23)12(2
InchiKey: BPGZBMINTWQDOH-UHFFFAOYSA-N
Formula: C12H4F14
SMILES: FC(F)(F)C(F)(c1ccc(C(F)(C(F)(F)F)C(F)(F)F)cc1)C(F)(F)F
Mol. weight [g/mol]: 414.14
CAS: 51114-12-6

Physical Properties

Property code	Value	Unit	Source
gf	-2557.36	kJ/mol	Joback Method
hf	-2863.99	kJ/mol	Joback Method
hfus	19.12	kJ/mol	Joback Method
hvap	26.03	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.265		Crippen Method
mcvol	180.960	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
tb	476.02	K	Joback Method
tc	621.47	K	Joback Method
tf	286.72	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.58	J/mol×K	476.02	Joback Method
cpg	490.51	J/mol×K	500.26	Joback Method
cpg	503.40	J/mol×K	524.50	Joback Method
cpg	515.30	J/mol×K	548.75	Joback Method
cpg	526.26	J/mol×K	572.99	Joback Method
cpg	536.34	J/mol×K	597.23	Joback Method
cpg	545.60	J/mol×K	621.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51114126&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume