2,6-Diisopropylfluorobenzene

Inchi: InChI=1S/C12H17F/c1-8(2)10-6-5-7-11(9(3)4)12(10)13/h5-9H,1-4H3
InchiKey: WAWGGRDKKRRDOY-UHFFFAOYSA-N
Formula: C12H17F
SMILES: CC(C)c1cccc(C(C)C)c1F
Mol. weight [g/mol]: 180.26
CAS: 87591-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-56.38	kJ/mol	Joback Method
hf	-284.09	kJ/mol	Joback Method
hfus	16.13	kJ/mol	Joback Method
hvap	44.31	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	4.072		Crippen Method
mcvol	157.950	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
tb	508.99	K	Joback Method
tc	709.13	K	Joback Method
tf	247.05	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.45	J/mol×K	508.99	Joback Method
cpg	371.64	J/mol×K	542.35	Joback Method
cpg	387.01	J/mol×K	575.70	Joback Method
cpg	401.59	J/mol×K	609.06	Joback Method
cpg	415.40	J/mol×K	642.41	Joback Method
cpg	428.47	J/mol×K	675.77	Joback Method
cpg	440.83	J/mol×K	709.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87591057&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

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