1,1,2-Trifluoro-1,2-diphenylethane

Inchi: InChI=1S/C14H11F3/c15-13(11-7-3-1-4-8-11)14(16,17)12-9-5-2-6-10-12/h1-10,13H
InchiKey: DSSQFJAXTVBOCK-UHFFFAOYSA-N
Formula: C14H11F3
SMILES: FC(c1ccccc1)C(F)(F)c1ccccc1
Mol. weight [g/mol]: 236.23
CAS: 68936-77-6

Physical Properties

Property code	Value	Unit	Source
chs	-7069.10 ± 1.90	kJ/mol	NIST Webbook
gf	-292.21	kJ/mol	Joback Method
hf	-462.20 ± 2.10	kJ/mol	NIST Webbook
hfs	-555.30 ± 1.90	kJ/mol	NIST Webbook
hfus	18.40	kJ/mol	Joback Method
hsub	93.13 ± 0.79	kJ/mol	NIST Webbook
hsub	93.10	kJ/mol	NIST Webbook
hvap	47.17	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.489		Crippen Method
mcvol	165.910	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
tb	567.22	K	Joback Method
tc	790.81	K	Joback Method
tf	289.57	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.93	J/mol×K	753.54	Joback Method
cpg	400.48	J/mol×K	567.22	Joback Method
cpg	417.11	J/mol×K	604.48	Joback Method
cpg	432.38	J/mol×K	641.75	Joback Method
cpg	446.37	J/mol×K	679.01	Joback Method

cpg	459.19	J/mol×K	716.28	Joback Method
cpg	481.66	J/mol×K	790.81	Joback Method
hfust	28.37	kJ/mol	354.20	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68936776&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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