

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]:	236.24

Physical Properties

Property code	Value	Unit	Source
chs	-7069.10 ± 1.90	kJ/mol	NIST Webbook
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	93.10	kJ/mol	NIST Webbook
hsub	93.13 ± 0.79	kJ/mol	NIST Webbook
hvap	73.88	kJ/mol	Cheméo Relay (1.0)
ie	9.09	eV	Cheméo Relay (1.0)
log10ws	-4.11		Cheméo Relay (1.0)
logp	4.489		Crippen Method
mcvol	165.910	ml/mol	McGowan Method
tb	536.36	K	Cheméo Relay (1.0)
tc	786.07	K	Cheméo Relay (1.0)
tf	352.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	470.93	J/mol×K	753.54	Joback Method
cpg	481.66	J/mol×K	790.81	Joback Method
hfust	28.37	kJ/mol	354.20	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68936776&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/14-089-8/1-1-2-TRIFLUORO-1-2-DIPHENYLETHANE.pdf>

Generated by Cheméo on 2026-07-21 21:13:28.493259275 +0000 UTC m=+179504.335144679.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.