Benzene, 1,2,4,5-tetrafluoro-3-(trifluoromethyl)-

Other names: Toluene, «alpha»,«alpha»,«alpha»,2,3,5,6-heptafluoro-
1-(Trifluoromethyl)-2,3,5,6-tetrafluorobenzene
4H-Heptafluorotoluene
«alpha»,«alpha»,«alpha»,2,3,5,6-Heptafluoro-toluene

Inchi: InChI=1S/C7HF7/c8-2-1-3(9)6(11)4(5(2)10)7(12,13)14/h1H

InchiKey: ZVPAJILXQHMKMT-UHFFFAOYSA-N

Formula: C7HF7

SMILES: Fc1cc(F)c(F)c(C(F)(F)F)c1F

Mol. weight [g/mol]: 218.07

CAS: 651-80-9

Physical Properties

Property code	Value	Unit	Source
gf	-1278.88	kJ/mol	Joback Method
hf	-1378.68	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	29.09	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.262		Crippen Method
mcvol	98.120	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
tb	384.70	K	NIST Webbook
tc	556.06	K	Joback Method
tf	251.70	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.39	J/mol×K	397.82	Joback Method
cpg	210.81	J/mol×K	424.19	Joback Method
cpg	217.86	J/mol×K	450.57	Joback Method
cpg	224.55	J/mol×K	476.94	Joback Method
cpg	230.88	J/mol×K	503.31	Joback Method

cpg	236.89	J/mol×K	529.69	Joback Method
cpg	242.56	J/mol×K	556.06	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=C651809&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume