Benzene, methyl-, trifluoro deriv.

Inchi: InChI=1S/C7H5F3/c8-4-5-2-1-3-6(9)7(5)10/h1-3H,4H2
InchiKey: QCUDEATVOVLIKY-UHFFFAOYSA-N
Formula: C7H5F3
SMILES: FCc1cccc(F)c1F
Mol. weight [g/mol]: 146.11
CAS: 27359-10-0

Physical Properties

Property code	Value	Unit	Source
chl	-3369.30 ± 0.50	kJ/mol	NIST Webbook
gf	-483.22	kJ/mol	Joback Method
hf	-562.55	kJ/mol	Joback Method
hfl	-636.70 ± 1.00	kJ/mol	NIST Webbook
hfus	16.39	kJ/mol	Joback Method
hvap	37.50	kJ/mol	NIST Webbook
log10ws	-2.87		Crippen Method
logp	2.434		Crippen Method
mcvol	91.040	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	394.01	K	Joback Method
tc	575.04	K	Joback Method
tf	221.88	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.84	J/mol×K	394.01	Joback Method
cpg	174.61	J/mol×K	424.18	Joback Method
cpg	182.97	J/mol×K	454.35	Joback Method
cpg	190.95	J/mol×K	484.53	Joback Method
cpg	198.54	J/mol×K	514.70	Joback Method
cpg	205.76	J/mol×K	544.87	Joback Method
cpg	212.62	J/mol×K	575.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27359100&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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