Trifluoromethyl (2-hydroxy-1-propenyl) ketone

Inchi: InChI=1S/C5H5F3O2/c1-3(9)2-4(10)5(6,7)8/h2,9H,1H3/b3-2-
InchiKey: GEGQNWRDBRXWDX-IHWYPQMZSA-N
Formula: C5H5F3O2
SMILES: CC(O)=CC(=O)C(F)(F)F
Mol. weight [g/mol]: 154.09
CAS: 7291-30-7

Physical Properties

Property code	Value	Unit	Source
gf	-784.44	kJ/mol	Joback Method
hf	-900.99	kJ/mol	Joback Method
hfus	15.11	kJ/mol	Joback Method
hvap	46.44	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.580		Crippen Method
mcvol	89.760	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
tb	458.47	K	Joback Method
tc	626.57	K	Joback Method
tf	232.40 ± 0.10	K	NIST Webbook
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.16	J/mol×K	542.52	Joback Method
cpg	221.01	J/mol×K	570.53	Joback Method
cpg	226.46	J/mol×K	598.55	Joback Method
cpg	195.06	J/mol×K	458.47	Joback Method
cpg	202.22	J/mol×K	486.49	Joback Method
cpg	208.91	J/mol×K	514.50	Joback Method
cpg	231.56	J/mol×K	626.57	Joback Method
hfust	8.45	kJ/mol	232.40	NIST Webbook
hfust	8.45	kJ/mol	232.40	NIST Webbook

sfust	36.40	J/mol×K	232.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7291307&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume