2,2,2-Trifluoroethyl radical

Inchi: InChI=1S/C2H2F3/c1-2(3,4)5/h1H2
InchiKey: COLOHWPRNRVWPI-UHFFFAOYSA-N
Formula: C2H2F3
SMILES: [CH2]C(F)(F)F
Mol. weight [g/mol]: 83.03
CAS: 3248-58-6

Physical Properties

Property code	Value	Unit	Source
gf	-563.25	kJ/mol	Joback Method
hf	-625.88	kJ/mol	Joback Method
hfus	4.44	kJ/mol	Joback Method
hvap	16.15	kJ/mol	Joback Method
ie	10.60 ± 0.10	eV	NIST Webbook
log10ws	-0.93		Crippen Method
logp	1.383		Crippen Method
mcvol	42.200	ml/mol	McGowan Method
pc	4553.06	kPa	Joback Method
tb	239.04	K	Joback Method
tc	375.04	K	Joback Method
tf	132.86	K	Joback Method
vc	0.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	57.50	J/mol×K	239.04	Joback Method
cpg	62.95	J/mol×K	261.71	Joback Method
cpg	68.04	J/mol×K	284.37	Joback Method
cpg	72.79	J/mol×K	307.04	Joback Method
cpg	77.21	J/mol×K	329.71	Joback Method
cpg	81.32	J/mol×K	352.37	Joback Method
cpg	85.13	J/mol×K	375.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3248586&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
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume