C3H3F3O2

Other names: 3,3,3-trifluoropropanoic acid
Inchi: InChI=1S/C3H3F3O2/c4-3(5,6)1-2(7)8/h1H2,(H,7,8)
InchiKey: KSNKQSPJFRQSEI-UHFFFAOYSA-N
Formula: C3H3F3O2
SMILES: O=C(O)CC(F)(F)F
Mol. weight [g/mol]: 128.05
CAS: 2516-99-6

Physical Properties

Property code	Value	Unit	Source
gf	-872.95	kJ/mol	Joback Method
hf	-967.14	kJ/mol	Joback Method
hfus	11.04	kJ/mol	Joback Method
hvap	41.95	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	1.023		Crippen Method
mcvol	65.880	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	418.70 ± 2.00	K	NIST Webbook
tc	567.78	K	Joback Method
tf	238.51	K	Joback Method
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.60	J/mol×K	408.67	Joback Method
cpg	143.98	J/mol×K	435.19	Joback Method
cpg	149.04	J/mol×K	461.71	Joback Method
cpg	153.81	J/mol×K	488.22	Joback Method
cpg	158.28	J/mol×K	514.74	Joback Method
cpg	162.48	J/mol×K	541.26	Joback Method
cpg	166.42	J/mol×K	567.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2516996&Units=SI

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