C4H5F3O2

Inchi: InChI=1S/C4H5F3O2/c5-4(6,7)2-1-3(8)9/h1-2H2,(H,8,9)
InchiKey: WTUCTMYLCMVYEX-UHFFFAOYSA-N
Formula: C4H5F3O2
SMILES: O=C(O)CCC(F)(F)F
Mol. weight [g/mol]: 142.08
CAS: 406-93-9

Physical Properties

Property code	Value	Unit	Source
gf	-864.53	kJ/mol	Joback Method
hf	-987.78	kJ/mol	Joback Method
hfus	13.63	kJ/mol	Joback Method
hvap	44.18	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.413		Crippen Method
mcvol	79.970	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
tb	431.55	K	Joback Method
tc	590.20	K	Joback Method
tf	249.78	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.17	J/mol×K	431.55	Joback Method
cpg	180.69	J/mol×K	457.99	Joback Method
cpg	186.84	J/mol×K	484.43	Joback Method
cpg	192.66	J/mol×K	510.88	Joback Method
cpg	198.15	J/mol×K	537.32	Joback Method
cpg	203.33	J/mol×K	563.76	Joback Method
cpg	208.21	J/mol×K	590.20	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=C406939&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