Ethyl 3-hydroxy-4,4,4-trifluorobutyrate

Other names: Butanoic acid, 4,4,4-trifluoro-3-hydroxy-, ethyl ester
Inchi: InChI=1S/C6H9F3O3/c1-2-12-5(11)3-4(10)6(7,8)9/h4,10H,2-3H2,1H3
InchiKey: ZWEDFBKLJILTMC-UHFFFAOYSA-N
Formula: C6H9F3O3
SMILES: CCOC(=O)CC(O)C(F)(F)F
Mol. weight [g/mol]: 186.13
CAS: 372-30-5

Physical Properties

Property code	Value	Unit	Source
gf	-955.13	kJ/mol	Joback Method
hf	-1166.56	kJ/mol	Joback Method
hfus	16.47	kJ/mol	Joback Method
hvap	50.65	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.863		Crippen Method
mcvol	114.020	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	499.29	K	Joback Method
tc	659.88	K	Joback Method
tf	279.55	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.25	J/mol×K	499.29	Joback Method
cpg	282.81	J/mol×K	526.06	Joback Method
cpg	290.97	J/mol×K	552.82	Joback Method
cpg	298.74	J/mol×K	579.59	Joback Method
cpg	306.14	J/mol×K	606.35	Joback Method
cpg	313.17	J/mol×K	633.12	Joback Method
cpg	319.84	J/mol×K	659.88	Joback Method

Sources

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=C372305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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