4-Hydroxy-6-oxohept-4-enoic acid, trifluoroacetate

Inchi: InChI=1S/C9H9F3O5/c1-5(13)4-6(2-3-7(14)15)17-8(16)9(10,11)12/h4H,2-3H2,1H3,(H,14

InchiKey: IFBOHNHOCRODNL-XQRVVYSFSA-N

Formula: C9H9F3O5

SMILES: CC(=O)C=C(CCC(=O)O)OC(=O)C(F)(F)F

Mol. weight [g/mol]: 254.16

Physical Properties

Property code	Value	Unit	Source
gf	-1113.60	kJ/mol	Joback Method
hf	-1340.93	kJ/mol	Joback Method
hfus	29.86	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.430		Crippen Method
mcvol	155.130	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1259.00		NIST Webbook
rinpol	1259.00		NIST Webbook
tb	680.15	K	Joback Method
tc	860.02	K	Joback Method
tf	409.18	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.37	J/mol×K	680.15	Joback Method
cpg	422.67	J/mol×K	710.13	Joback Method
cpg	430.44	J/mol×K	740.11	Joback Method
cpg	437.71	J/mol×K	770.09	Joback Method
cpg	444.50	J/mol×K	800.06	Joback Method
cpg	450.86	J/mol×K	830.04	Joback Method
cpg	456.79	J/mol×K	860.02	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=U374327&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume