Propionic acid, 2,3,3,3-tetrafluoro-, ethyl ester

Inchi: InChI=1S/C5H6F4O2/c1-2-11-4(10)3(6)5(7,8)9/h3H,2H2,1H3
InchiKey: YJROLMPBFOAPOX-UHFFFAOYSA-N
Formula: C5H6F4O2
SMILES: CCOC(=O)C(F)C(F)(F)F
Mol. weight [g/mol]: 174.09
CAS: 399-92-8

Physical Properties

Property code	Value	Unit	Source
gf	-1021.54	kJ/mol	Joback Method
hf	-1189.80	kJ/mol	Joback Method
hfus	12.88	kJ/mol	Joback Method
hvap	30.93	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.450		Crippen Method
mcvol	95.830	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
tb	383.50	K	Joback Method
tc	540.33	K	Joback Method
tf	208.05	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.27	J/mol×K	383.50	Joback Method
cpg	206.60	J/mol×K	409.64	Joback Method
cpg	214.57	J/mol×K	435.78	Joback Method
cpg	222.19	J/mol×K	461.92	Joback Method
cpg	229.47	J/mol×K	488.06	Joback Method
cpg	236.41	J/mol×K	514.19	Joback Method
cpg	243.02	J/mol×K	540.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C399928&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
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