ETHYL 4,4,4-TRIFLUOROACETOACETATE

Other names:	4,4,4-Trifluoro-3-oxobutanoic acid ethyl ester
	4,4,4-Trifluoroacetoacetic acid ethyl ester
	Acetoacetic acid, 4,4,4-trifluoro-, ethyl ester
	Acetoacetic acid, 4-trifluoro-, ethyl ester
	Ethyl (trifluoroacetyl)acetate
	Ethyl 4,4,4-trifluoro-3-oxobutanoate
	Ethyl 4,4,4-trifluoro-3-oxobutyrate
	Ethyl 4,4,4-trifluoroacetoacetate
	Ethyl trifluoroacetoacetate
	Ethyl «gamma»,«gamma»,«gamma»-trifluoroacetoacetate
	Ethyl «omega»,«omega»,«omega»-trifluoroacetoacetate
	NSC 42739
Inchi:	InChI=1S/C6H7F3O3/c1-2-12-5(11)3-4(10)6(7,8)9/h2-3H2,1H3
InchiKey:	OCJKUQIPRNZDTK-UHFFFAOYSA-N
Formula:	C6H7F3O3
SMILES:	CCOC(=O)CC(=O)C(F)(F)F
Mol. weight [g/mol]:	184.11

Physical Properties

Property code	Value	Unit	Source
af	0.4030		Cheméo Relay (1.0)
gf	-944.79	kJ/mol	Joback Method
hf	-1216.97	kJ/mol	Cheméo Relay (1.0)
hfus	17.51	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Cheméo Relay (1.0)
ie	10.33	eV	Cheméo Relay (1.0)
log10ws	-0.91		Cheméo Relay (1.0)
logp	1.071		Crippen Method
mcvol	109.720	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
tb	402.70	K	NIST Webbook
tb	402.50 ± 0.50	K	NIST Webbook
tc	538.13	K	Cheméo Relay (1.0)
tf	234.77	K	Cheméo Relay (1.0)
vc	0.388	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.19	J/mol×K	461.42	Joback Method
cpg	252.10	J/mol×K	490.14	Joback Method
cpg	260.58	J/mol×K	518.85	Joback Method
cpg	268.64	J/mol×K	547.57	Joback Method
cpg	276.28	J/mol×K	576.28	Joback Method
cpg	283.52	J/mol×K	605.00	Joback Method
cpg	290.37	J/mol×K	633.71	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C372316&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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

ie: Ionization energy

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