

Butanoic acid, 4,4,4-trifluoro-3-oxo-, ethyl ester

Other names:	Ethyl trifluoroacetoacetate
	Ethyl 4,4,4-trifluoroacetoacetate
	Ethyl «gamma»,«gamma»,«gamma»-trifluoroacetoacetate
	4,4,4-Trifluoroacetoacetic acid ethyl ester
	Ethyl «omega»,«omega»,«omega»-trifluoroacetoacetate
	Acetoacetic acid, 4,4,4-trifluoro-, ethyl ester
	Ethyl (trifluoroacetyl)acetate
	Acetoacetic acid, 4-trifluoro-, ethyl ester
	Ethyl 4,4,4-trifluoro-3-oxobutanoate
	Ethyl 4,4,4-trifluoro-3-oxobutyrate
	NSC 42739
	4,4,4-Trifluoro-3-oxobutanoic acid ethyl ester
	InChI=1S/C6H7F3O3/c1-2-12-5(11)3-4(10)6(7,8)9/h2-3H2,1H3
Inchi:	
InchiKey:	OCJKUQIPRNZDTK-UHFFFAOYSA-N
Formula:	C6H7F3O3
SMILES:	CCOC(=O)CC(=O)C(F)(F)F
Mol. weight [g/mol]:	184.11
CAS:	372-31-6

Physical Properties

Property code	Value	Unit	Source
gf	-944.79	kJ/mol	Joback Method
hf	-1121.63	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	41.10	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
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	633.71	K	Joback Method
tf	283.66	K	Joback Method
vc	0.445	m3/kmol	Joback Method

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

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

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

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