ETHYL 4,4,4-TRIFLUOROCROTONATE

Other names: 2-Butenoic acid, 4,4,4-trifluoro-, ethyl ester, (2E)-
ETHYL-4,4,4-TRIFLUORO-2-BUTENOATE
Inchi: InChI=1S/C6H7F3O2/c1-2-11-5(10)3-4-6(7,8)9/h3-4H,2H2,1H3
InchiKey: ZKRJCMKLCDWROR-ONEGZZNKSA-N
Formula: C6H7F3O2
SMILES: CCOC(=O)/C=C/C(F)(F)F
Mol. weight [g/mol]: 168.11

Physical Properties

Property code	Value	Unit	Source
af	0.3769		Cheméo Relay (1.0)
hf	-1029.95	kJ/mol	Cheméo Relay (1.0)
hfus	16.11	kJ/mol	Joback Method
hvap	45.75	kJ/mol	Cheméo Relay (1.0)
ie	10.75	eV	Cheméo Relay (1.0)
log10ws	-2.34		Cheméo Relay (1.0)
logp	1.668		Crippen Method
mcvol	103.850	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	388.17	K	Cheméo Relay (1.0)
tc	543.07	K	Cheméo Relay (1.0)
tf	239.89	K	Cheméo Relay (1.0)
vc	0.370	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.48	J/mol×K	411.71	Joback Method
cpg	220.77	J/mol×K	439.92	Joback Method
cpg	229.57	J/mol×K	468.14	Joback Method
cpg	237.91	J/mol×K	496.35	Joback Method
cpg	245.80	J/mol×K	524.57	Joback Method
cpg	253.26	J/mol×K	552.78	Joback Method
cpg	260.31	J/mol×K	580.99	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25597164&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
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