Ethyl-4,4,4-trifluoro-3-(trifluoromethyl)crotonate

Inchi: InChI=1S/C7H6F6O2/c1-2-15-5(14)3-4(6(8,9)10)7(11,12)13/h3H,2H2,1H3
InchiKey: CULZFNOUPBWSIZ-UHFFFAOYSA-N
Formula: C7H6F6O2
SMILES: CCOC(=O)C=C(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 236.11

Physical Properties

Property code	Value	Unit	Source
af	0.4252		Cheméo Relay (1.0)
hf	-1616.28	kJ/mol	Cheméo Relay (1.0)
hfus	19.22	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Cheméo Relay (1.0)
ie	10.88	eV	Cheméo Relay (1.0)
log10ws	-3.30		Cheméo Relay (1.0)
logp	2.601		Crippen Method
mcvol	123.250	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
tb	392.28	K	Cheméo Relay (1.0)
tc	526.44	K	Cheméo Relay (1.0)
tf	183.06	K	Cheméo Relay (1.0)
vc	0.452	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.30	J/mol×K	429.05	Joback Method
cpg	287.47	J/mol×K	455.14	Joback Method
cpg	297.04	J/mol×K	481.24	Joback Method
cpg	306.05	J/mol×K	507.33	Joback Method
cpg	314.52	J/mol×K	533.43	Joback Method
cpg	322.48	J/mol×K	559.52	Joback Method
cpg	329.94	J/mol×K	585.62	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1513606&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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