2,2,2-TRIFLUORO-1-(TRIFLUOROMETHYL)ETHYL ACRYLATE

Other names: 2-Propenoic acid, 2,2,2-trifluoro-1-(trifluoromethyl)ethyl ester
1,1,1,3,3,3-Hexafluoroisopropyl acrylate
2,2,2-trifluoro-1-(trifluoromethyl)ethyl acrylate

Inchi: InChI=1S/C6H4F6O2/c1-2-3(13)14-4(5(7,8)9)6(10,11)12/h2,4H,1H2

InchiKey: MNSWITGNWZSAMC-UHFFFAOYSA-N

Formula: C6H4F6O2

SMILES: C=CC(=O)OC(C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 222.08

Physical Properties

Property code	Value	Unit	Source
hfus	12.93	kJ/mol	Joback Method
logp	2.209		Crippen Method
mcvol	109.160	ml/mol	McGowan Method
tb	357.50 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.62	J/mol×K	398.37	Joback Method
cpg	247.81	J/mol×K	423.87	Joback Method
cpg	256.49	J/mol×K	449.37	Joback Method
cpg	264.67	J/mol×K	474.88	Joback Method
cpg	272.36	J/mol×K	500.38	Joback Method
cpg	279.60	J/mol×K	525.88	Joback Method
cpg	286.39	J/mol×K	551.38	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=C2160896&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature