2,2,2-Trifluoroethyl methacrylate

Other names:	Trifluoroethyl methacrylate
	Methacrylic acid 2,2,2-trifluoroethyl ester
	2-Propenoic acid, 2-methyl-, 2,2,2-trifluoroethyl ester
Inchi:	InChI=1S/C6H7F3O2/c1-4(2)5(10)11-3-6(7,8)9/h1,3H2,2H3
InchiKey:	QTKPMCIBUROOGY-UHFFFAOYSA-N
Formula:	C6H7F3O2
SMILES:	C=C(C)C(=O)OCC(F)(F)F
Mol. weight [g/mol]:	168.11
CAS:	352-87-4

Physical Properties

Property code	Value	Unit	Source
gf	-736.58	kJ/mol	Joback Method
hf	-893.41	kJ/mol	Joback Method
hfus	13.32	kJ/mol	Joback Method
hvap	33.77	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.668		Crippen Method
mcvol	103.850	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	404.11	K	Joback Method
tc	571.76	K	Joback Method
tf	218.01	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.90	J/mol×K	404.11	Joback Method
cpg	221.07	J/mol×K	432.05	Joback Method
cpg	229.79	J/mol×K	459.99	Joback Method
cpg	238.08	J/mol×K	487.94	Joback Method
cpg	245.95	J/mol×K	515.88	Joback Method
cpg	253.43	J/mol×K	543.82	Joback Method

cpg	260.51	J/mol×K	571.76	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	303.00	K	5.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C352874&Units=SI
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

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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