

2,2,2-TRIFLUOROETHYL ACRYLATE

Other names:	2-Propenoic acid, 2,2,2-trifluoroethyl ester Acrylic acid, 2,2,2-trifluoroethyl ester
Inchi:	InChI=1S/C5H5F3O2/c1-2-4(9)10-3-5(6,7)8/h2H,1,3H2
InchiKey:	VBHXIMACZBQHPX-UHFFFAOYSA-N
Formula:	C5H5F3O2
SMILES:	C=CC(=O)OCC(F)(F)F
Mol. weight [g/mol]:	154.09

Physical Properties

Property code	Value	Unit	Source
af	0.4159		Cheméo Relay (1.0)
hf	-970.46	kJ/mol	Cheméo Relay (1.0)
hfus	12.04	kJ/mol	Joback Method
hvap	38.66	kJ/mol	Cheméo Relay (1.0)
ie	11.25	eV	Cheméo Relay (1.0)
log10ws	-0.90		Cheméo Relay (1.0)
logp	1.278		Crippen Method
mcvol	89.760	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	366.51	K	Cheméo Relay (1.0)
tc	529.73	K	Cheméo Relay (1.0)
tf	231.33	K	Cheméo Relay (1.0)
vc	0.321	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.99	J/mol×K	381.35	Joback Method
cpg	183.82	J/mol×K	408.84	Joback Method
cpg	191.27	J/mol×K	436.33	Joback Method
cpg	198.35	J/mol×K	463.83	Joback Method
cpg	205.08	J/mol×K	491.32	Joback Method
cpg	211.46	J/mol×K	518.81	Joback Method
cpg	217.50	J/mol×K	546.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	319.20	K	16.70	NIST Webbook
tbrp	319.00	K	16.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C407476&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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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

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