

1H,1H-Pentafluoro-n-propyl acrylate

Other names:	2,2,3,3,3-Pentafluoropropyl acrylate 2-Propenoic acid, 2,2,3,3,3-pentafluoropropyl ester
Inchi:	InChI=1S/C6H5F5O2/c1-2-4(12)13-3-5(7,8)6(9,10)11/h2H,1,3H2
InchiKey:	JDVGNKIUXZQTFD-UHFFFAOYSA-N
Formula:	C6H5F5O2
SMILES:	C=CC(=O)OCC(F)(F)C(F)(F)F
Mol. weight [g/mol]:	204.09

Physical Properties

Property code	Value	Unit	Source
af	0.4411		Cheméo Relay (1.0)
hf	-1382.94	kJ/mol	Cheméo Relay (1.0)
hfus	13.37	kJ/mol	Joback Method
hvap	41.24	kJ/mol	Cheméo Relay (1.0)
ie	11.24	eV	Cheméo Relay (1.0)
log10ws	-2.32		Cheméo Relay (1.0)
logp	1.913		Crippen Method
mcvol	107.390	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
tb	373.68	K	Cheméo Relay (1.0)
tc	508.77	K	Cheméo Relay (1.0)
tf	225.64	K	Cheméo Relay (1.0)
vc	0.384	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.37	J/mol×K	399.54	Joback Method
cpg	239.70	J/mol×K	425.80	Joback Method
cpg	248.50	J/mol×K	452.07	Joback Method
cpg	256.79	J/mol×K	478.33	Joback Method
cpg	264.59	J/mol×K	504.60	Joback Method
cpg	271.92	J/mol×K	530.86	Joback Method
cpg	278.79	J/mol×K	557.13	Joback Method

Sources

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=C356865&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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