PROPANOIC ACID, PENTAFLUORO-

Other names: 2,2,3,3,3-Pentafluoropropionic acid
Propanoic acid, pentafluoro-
Propionic acid, pentafluoro-
Inchi: InChI=1S/C3HF5O2/c4-2(5,1(9)10)3(6,7)8/h(H,9,10)
InchiKey: LRMSQVBRUNSOJL-UHFFFAOYSA-N
Formula: C3HF5O2
SMILES: O=C(O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 164.03

Physical Properties

Property code	Value	Unit	Source
hf	-1487.51	kJ/mol	Cheméo Relay (1.0)
hfus	9.78	kJ/mol	Joback Method
hvap	47.52	kJ/mol	Cheméo Relay (1.0)
ie	12.25	eV	Cheméo Relay (1.0)
logp	1.269		Crippen Method
mcvol	69.420	ml/mol	McGowan Method
rinpol	781.00		NIST Webbook
rinpol	781.00		NIST Webbook
tb	369.50 ± 0.50	K	NIST Webbook
tb	370.00 ± 1.00	K	NIST Webbook
tb	370.07 ± 0.20	K	NIST Webbook
tf	307.59	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.76	J/mol×K	403.98	Joback Method
cpg	163.55	J/mol×K	429.40	Joback Method
cpg	168.91	J/mol×K	454.83	Joback Method
cpg	173.88	J/mol×K	480.25	Joback Method
cpg	178.47	J/mol×K	505.67	Joback Method
cpg	182.70	J/mol×K	531.10	Joback Method
cpg	186.59	J/mol×K	556.52	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=C422640&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point