

Propanal, pentafluoro-

Other names:	Propionaldehyde, pentafluoro- Pentafluoropropionaldehyde Perfluoropropionaldehyde
Inchi:	InChI=1S/C3HF5O/c4-2(5,1-9)3(6,7)8/h1H
InchiKey:	IRPGOXJVTQTAAN-UHFFFAOYSA-N
Formula:	C3HF5O
SMILES:	O=CC(F)(F)C(F)(F)F
Mol. weight [g/mol]:	148.03
CAS:	422-06-0

Physical Properties

Property code	Value	Unit	Source
gf	-1093.51	kJ/mol	Joback Method
hf	-1188.88	kJ/mol	Joback Method
hfus	6.39	kJ/mol	Joback Method
hvap	22.32	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.383		Crippen Method
mcvol	63.550	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
tb	275.00 ± 3.00	K	NIST Webbook
tc	453.77	K	Joback Method
tf	173.36	K	Joback Method
vc	0.288	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	122.17	J/mol×K	306.59	Joback Method
cpg	128.97	J/mol×K	331.12	Joback Method
cpg	135.33	J/mol×K	355.65	Joback Method
cpg	141.27	J/mol×K	380.18	Joback Method
cpg	146.81	J/mol×K	404.71	Joback Method
cpg	151.96	J/mol×K	429.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C422060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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