Pentafluoropropionamide

Other names:	Propanamide, 2,2,3,3,3-pentafluoro- 2,2,3,3,3-pentafluoropropionamide
Inchi:	InChI=1S/C3H2F5NO/c4-2(5,1(9)10)3(6,7)8/h(H2,9,10)
InchiKey:	KQTOYEUYHXUEDB-UHFFFAOYSA-N
Formula:	C3H2F5NO
SMILES:	NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	163.05
CAS:	354-76-7

Physical Properties

Property code	Value	Unit	Source
gf	-1056.46	kJ/mol	Joback Method
hf	-1182.09	kJ/mol	Joback Method
hfus	10.89	kJ/mol	Joback Method
hvap	32.98	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	0.669		Crippen Method
mcvol	73.530	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	384.33	K	Joback Method
tc	554.27	K	Joback Method
tf	264.55	K	Joback Method
vc	0.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.07	J/mol×K	384.33	Joback Method
cpg	170.37	J/mol×K	412.65	Joback Method
cpg	177.12	J/mol×K	440.98	Joback Method
cpg	183.34	J/mol×K	469.30	Joback Method
cpg	189.07	J/mol×K	497.63	Joback Method
cpg	194.32	J/mol×K	525.95	Joback Method
cpg	199.13	J/mol×K	554.27	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C354767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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