Propyne, 3-fluoro-

Inchi: InChI=1S/C3H3F/c1-2-3-4/h1H,3H2
InchiKey: QEMMTKPYWRKLME-UHFFFAOYSA-N
Formula: C3H3F
SMILES: C#CCF
Mol. weight [g/mol]: 58.05
CAS: 2805-22-3

Physical Properties

Property code	Value	Unit	Source
gf	2.64	kJ/mol	Joback Method
hf	-9.46	kJ/mol	Joback Method
hfus	9.58	kJ/mol	Joback Method
hvap	21.31	kJ/mol	Joback Method
ie	10.95	eV	NIST Webbook
log10ws	-0.73		Crippen Method
logp	0.589		Crippen Method
mcvol	46.300	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
tb	257.43	K	Joback Method
tc	417.72	K	Joback Method
tf	171.13	K	Joback Method
vc	0.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	64.01	J/mol×K	257.43	Joback Method
cpg	67.63	J/mol×K	284.14	Joback Method
cpg	71.08	J/mol×K	310.86	Joback Method
cpg	74.38	J/mol×K	337.57	Joback Method
cpg	77.54	J/mol×K	364.29	Joback Method
cpg	80.55	J/mol×K	391.00	Joback Method
cpg	83.43	J/mol×K	417.72	Joback Method

Sources

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=C2805223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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