

1,2,2-trifluoroethyl

Inchi:

InChI=1S/C2H2F3/c3-1-2(4)5/h1-2H

InchiKey:

GGNPAIXDALWWEI-UHFFFAOYSA-N

Formula:

C2H2F3

SMILES:

F[CH]C(F)F

Mol. weight [g/mol]:

83.03

CAS:

116819-06-8

Physical Properties

Property code	Value	Unit	Source
gf	-570.97	kJ/mol	Joback Method
hf	-627.69	kJ/mol	Joback Method
hfus	4.81	kJ/mol	Joback Method
hvap	16.67	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	1.383		Crippen Method
mcvol	42.200	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
tb	241.39	K	Joback Method
tc	375.17	K	Joback Method
tf	100.44	K	Joback Method
vc	0.180	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	60.28	J/mol×K	241.39	Joback Method
cpg	64.62	J/mol×K	263.69	Joback Method
cpg	68.72	J/mol×K	285.98	Joback Method
cpg	72.59	J/mol×K	308.28	Joback Method
cpg	76.24	J/mol×K	330.58	Joback Method
cpg	79.68	J/mol×K	352.87	Joback Method
cpg	82.92	J/mol×K	375.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C116819068&Units=SI

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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