

Propane, 2,3,3-trichloro-1,1,1-trifluoro-

Inchi:	InChI=1S/C3H2Cl3F3/c4-1(2(5)6)3(7,8)9/h1-2H
InchiKey:	UHUGFVKSZJCZEY-UHFFFAOYSA-N
Formula:	C3H2Cl3F3
SMILES:	FC(F)(F)C(Cl)C(Cl)Cl
Mol. weight [g/mol]:	201.40
CAS:	431-51-6

Physical Properties

Property code	Value	Unit	Source
gf	-647.88	kJ/mol	Joback Method
hf	-760.11	kJ/mol	Joback Method
hfus	10.90	kJ/mol	Joback Method
hvap	30.90	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.960		Crippen Method
mcvol	95.160	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	374.03	K	Joback Method
tc	555.13	K	Joback Method
tf	187.52	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.03	J/molxK	374.03	Joback Method
cpg	163.44	J/molxK	404.21	Joback Method
cpg	169.38	J/molxK	434.40	Joback Method
cpg	174.87	J/molxK	464.58	Joback Method
cpg	179.93	J/molxK	494.76	Joback Method
cpg	184.59	J/molxK	524.95	Joback Method
cpg	188.87	J/molxK	555.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C431516&Units=SI
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

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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