1,1,1-Trifluoro-3-methylbutane

Inchi: InChI=1S/C5H9F3/c1-4(2)3-5(6,7)8/h4H,3H2,1-2H3
InchiKey: CONTVCYXDSFGMN-UHFFFAOYSA-N
Formula: C5H9F3
SMILES: CC(C)CC(F)(F)F
Mol. weight [g/mol]: 126.12
CAS: 406-49-5

Physical Properties

Property code	Value	Unit	Source
gf	-592.81	kJ/mol	Joback Method
hf	-748.89	kJ/mol	Joback Method
hfus	7.01	kJ/mol	Joback Method
hvap	22.59	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.595		Crippen Method
mcvol	86.620	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	304.00	K	NIST Webbook
tc	457.45	K	Joback Method
tf	135.30	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.56	J/mol×K	307.94	Joback Method
cpg	158.16	J/mol×K	332.86	Joback Method
cpg	167.35	J/mol×K	357.78	Joback Method
cpg	176.12	J/mol×K	382.70	Joback Method
cpg	184.51	J/mol×K	407.61	Joback Method
cpg	192.52	J/mol×K	432.53	Joback Method
cpg	200.16	J/mol×K	457.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C406495&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