Butane, 1,1,1,2,3,3,4,4,4-nonafluoro-2-(trifluoromethyl)-

Other names: Butane, nonafluoro-2-(trifluoromethyl)-
Perfluoro-2-methylbutane

Inchi: InChI=1S/C5F12/c6-1(3(9,10)11,4(12,13)14)2(7,8)5(15,16)17

InchiKey: MPEFSWGYIJNMCW-UHFFFAOYSA-N

Formula: C5F12

SMILES: FC(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 288.03

CAS: 594-91-2

Physical Properties

Property code	Value	Unit	Source
gf	-2332.30	kJ/mol	Joback Method
hf	-2543.60	kJ/mol	Joback Method
hfus	8.60	kJ/mol	Joback Method
hvap	26.30	kJ/mol	NIST Webbook
hvap	27.40	kJ/mol	NIST Webbook
log10ws	-4.18		Crippen Method
logp	4.017		Crippen Method
mcvol	102.550	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
tb	288.89	K	Joback Method
tc	402.87	K	Joback Method
tf	165.29	K	Joback Method
tt	175.35 ± 0.30	K	NIST Webbook
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.40	J/mol×K	383.87	Joback Method
cpg	212.63	J/mol×K	288.89	Joback Method
cpg	224.00	J/mol×K	307.89	Joback Method
cpg	234.73	J/mol×K	326.88	Joback Method
cpg	244.87	J/mol×K	345.88	Joback Method

cpg	254.41	J/mol×K	364.88	Joback Method
cpg	271.83	J/mol×K	402.87	Joback Method
hvapt	31.00	kJ/mol	268.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38271e+01
Coeff. B	-2.31947e+03
Coeff. C	-5.14040e+01
Temperature range (K), min.	222.72
Temperature range (K), max.	323.78

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1615.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C594912&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume