butane, octafluoro-2,3-bis(trifluoromethyl)-

Other names: Perfluoro-2,3-dimethylbutane
Inchi: InChI=1S/C6F14/c7-1(3(9,10)11,4(12,13)14)2(8,5(15,16)17)6(18,19)20
InchiKey: NBQYGIPVNCVJJP-UHFFFAOYSA-N
Formula: C6F14
SMILES: FC(F)(F)C(F)(C(F)(F)F)C(F)(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 338.04
CAS: 354-96-1

Physical Properties

Property code	Value	Unit	Source
af	0.3940		KDB
gf	-2710.66	kJ/mol	Joback Method
hf	-2965.21	kJ/mol	Joback Method
hfus	9.93	kJ/mol	Joback Method
hvap	31.60	kJ/mol	NIST Webbook
log10ws	-4.91		Crippen Method
logp	4.652		Crippen Method
mcvol	120.180	ml/mol	McGowan Method
pc	1870.00	kPa	KDB
tb	332.93	K	KDB
tc	463.00	K	KDB
tf	180.16	K	Joback Method
tt	258.05 ± 0.30	K	NIST Webbook
vc	0.525	m3/kmol	KDB
zc	0.2550250		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.70	J/mol×K	307.08	Joback Method
cpg	276.21	J/mol×K	325.58	Joback Method
cpg	288.03	J/mol×K	344.08	Joback Method
cpg	299.18	J/mol×K	362.58	Joback Method
cpg	309.69	J/mol×K	381.08	Joback Method

cpg	319.57	J/mol×K	399.58	Joback Method
cpg	328.86	J/mol×K	418.08	Joback Method
hvapt	33.00	kJ/mol	297.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58930e+01
Coeff. B	-3.32601e+03
Coeff. C	-3.37100e+01
Temperature range (K), min.	246.84
Temperature range (K), max.	348.03

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.68275e+01
Coeff. B	-5.91833e+03
Coeff. C	-7.74489e+00
Coeff. D	4.88877e-06
Temperature range (K), min.	262.00
Temperature range (K), max.	452.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1630

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1630

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C354961&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
zc:	Critical Compressibility