1-Propene, 1,1,3,3,3-pentafluoro-2-(trifluoromethyl)-

Other names: 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)propene
1,1-Difluoro-2,2-bis(trifluoromethyl)ethene
Isobutene, octafluoro-
Octafluoro-sec-butene
Octafluoroisobutene
Octafluoroisobutylene
PFIB
Perfluorisobutylene
Perfluoro-2-(trifluoromethyl)propene
Perfluoro-2-methylpropene
Perfluoroisobutene
Perfluoroisobutylene
Propene, 1,1,3,3,3-pentafluoro-2-(trifluoromethyl)-
Propene, pentafluoro-2-(trifluoromethyl)-

Inchi: InChI=1S/C4F8/c5-2(6)1(3(7,8)9)4(10,11)12

InchiKey: DAFIBNSJXIGBQB-UHFFFAOYSA-N

Formula: C4F8

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

Mol. weight [g/mol]: 200.03

CAS: 382-21-8

Physical Properties

Property code	Value	Unit	Source
hf	-1577.85	kJ/mol	Cheméo Relay (1.0)
hfus	13.51	kJ/mol	Joback Method
hvap	19.70	kJ/mol	Cheméo Relay (1.0)
ie	10.99	eV	Cheméo Relay (1.0)
logp	3.262		Crippen Method
mcvol	77.080	ml/mol	McGowan Method
tb	274.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	143.06	J/mol×K	282.54	Joback Method
cpg	151.05	J/mol×K	303.75	Joback Method
cpg	158.59	J/mol×K	324.97	Joback Method
cpg	165.70	J/mol×K	346.18	Joback Method
cpg	172.38	J/mol×K	367.39	Joback Method
cpg	178.65	J/mol×K	388.60	Joback Method
cpg	184.53	J/mol×K	409.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63442e+01
Coeff. B	-2.94460e+03
Coeff. C	-1.90320e+01
Temperature range (K), min.	202.42
Temperature range (K), max.	299.15

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C382218&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature