

1,1,1-trifluorooctane

Inchi:	InChI=1S/C8H15F3/c1-2-3-4-5-6-7-8(9,10)11/h2-7H2,1H3
InchiKey:	FHMDVJKRMUAZOO-UHFFFAOYSA-N
Formula:	C8H15F3
SMILES:	CCCCCCCC(F)(F)F
Mol. weight [g/mol]:	168.20
CAS:	53392-86-2

Physical Properties

Property code	Value	Unit	Source
af	0.4588		Cheméo Relay (1.0)
gf	-565.11	kJ/mol	Joback Method
hf	-853.18	kJ/mol	Cheméo Relay (1.0)
hfus	18.30	kJ/mol	Joback Method
hvap	36.30	kJ/mol	Cheméo Relay (1.0)
ie	11.00	eV	Cheméo Relay (1.0)
log10ws	-4.19		Cheméo Relay (1.0)
logp	3.909		Crippen Method
mcvol	128.890	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
tb	387.45	K	Cheméo Relay (1.0)
tc	521.34	K	Cheméo Relay (1.0)
tf	183.66	K	Cheméo Relay (1.0)
vc	0.497	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.53	J/mol×K	377.02	Joback Method
cpg	270.17	J/mol×K	401.75	Joback Method
cpg	282.29	J/mol×K	426.48	Joback Method
cpg	293.91	J/mol×K	451.21	Joback Method
cpg	305.04	J/mol×K	475.94	Joback Method
cpg	315.70	J/mol×K	500.67	Joback Method
cpg	325.90	J/mol×K	525.40	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.27707e+01
Coeff. B	-3.00035e+03
Coeff. C	-5.26000e+01
Temperature range (K), min.	292.95
Temperature range (K), max.	454.84

Sources

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
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=C53392862&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ie:	Ionization energy
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
vc:	Critical Volume

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