

1-chloro-6-fluorohexane

Inchi:	InChI=1S/C6H12ClF/c7-5-3-1-2-4-6-8/h1-6H2
InchiKey:	NASMVDMHYMZBIM-UHFFFAOYSA-N
Formula:	C6H12ClF
SMILES:	FCCCCCCI
Mol. weight [g/mol]:	138.61
CAS:	1550-09-0

Physical Properties

Property code	Value	Unit	Source
af	0.4593		Cheméo Relay (1.0)
hf	-356.51	kJ/mol	Cheméo Relay (1.0)
hfus	18.57	kJ/mol	Joback Method
hvap	46.54	kJ/mol	Cheméo Relay (1.0)
ie	10.61	eV	Cheméo Relay (1.0)
log10ws	-3.03		Cheméo Relay (1.0)
logp	2.755		Crippen Method
mcvol	109.410	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
tb	423.13	K	Cheméo Relay (1.0)
tc	618.72	K	Cheméo Relay (1.0)
tf	237.80	K	Cheméo Relay (1.0)
vc	0.429	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.18	J/mol×K	373.38	Joback Method
cpg	204.06	J/mol×K	400.55	Joback Method
cpg	213.56	J/mol×K	427.73	Joback Method
cpg	222.71	J/mol×K	454.90	Joback Method
cpg	231.50	J/mol×K	482.08	Joback Method
cpg	239.96	J/mol×K	509.25	Joback Method
cpg	248.08	J/mol×K	536.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.62465e+01
Coeff. B	-4.29502e+03
Coeff. C	-6.37900e+01
Temperature range (K), min.	332.92
Temperature range (K), max.	456.57

Sources

The Yaws Handbook of Vapor Pressure:
Joback Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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
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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