

1-chloro-5-fluoropentane

Inchi:	InChI=1S/C5H10ClF/c6-4-2-1-3-5-7/h1-5H2
InchiKey:	HMHFNUWREZQHGX-UHFFFAOYSA-N
Formula:	C5H10ClF
SMILES:	FCCCCCl
Mol. weight [g/mol]:	124.59
CAS:	407-98-7

Physical Properties

Property code	Value	Unit	Source
af	0.4132		Cheméo Relay (1.0)
hf	-333.60	kJ/mol	Cheméo Relay (1.0)
hfus	15.98	kJ/mol	Joback Method
hvap	41.74	kJ/mol	Cheméo Relay (1.0)
ie	10.73	eV	Cheméo Relay (1.0)
log10ws	-2.38		Cheméo Relay (1.0)
logp	2.365		Crippen Method
mcvol	95.320	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	400.56	K	Cheméo Relay (1.0)
tc	594.49	K	Cheméo Relay (1.0)
tf	221.72	K	Cheméo Relay (1.0)
vc	0.371	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.36	J/mol×K	350.50	Joback Method
cpg	167.92	J/mol×K	377.67	Joback Method
cpg	176.15	J/mol×K	404.84	Joback Method
cpg	184.09	J/mol×K	432.01	Joback Method
cpg	191.72	J/mol×K	459.17	Joback Method
cpg	199.06	J/mol×K	486.34	Joback Method
cpg	206.11	J/mol×K	513.51	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.66240e+01
Coeff. B	-4.18514e+03
Coeff. C	-5.68950e+01
Temperature range (K), min.	313.08
Temperature range (K), max.	426.85

Sources

Cheméo Relay (1.0, beta):

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):

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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