

1-chloro-4-fluorobutane

Inchi:	InChI=1S/C4H8ClF/c5-3-1-2-4-6/h1-4H2
InchiKey:	RYKUJAHSVIVAQV-UHFFFAOYSA-N
Formula:	C4H8ClF
SMILES:	FCCCCCl
Mol. weight [g/mol]:	110.56
CAS:	462-73-7

Physical Properties

Property code	Value	Unit	Source
af	0.3643		Cheméo Relay (1.0)
hf	-311.73	kJ/mol	Cheméo Relay (1.0)
hfus	13.39	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Cheméo Relay (1.0)
ie	10.89	eV	Cheméo Relay (1.0)
log10ws	-1.72		Cheméo Relay (1.0)
logp	1.975		Crippen Method
mcvol	81.230	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	374.63	K	Cheméo Relay (1.0)
tc	566.29	K	Cheméo Relay (1.0)
tf	205.18	K	Cheméo Relay (1.0)
vc	0.314	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.11	J/mol×K	327.62	Joback Method
cpg	134.23	J/mol×K	354.72	Joback Method
cpg	141.10	J/mol×K	381.81	Joback Method
cpg	147.71	J/mol×K	408.91	Joback Method
cpg	154.07	J/mol×K	436.00	Joback Method
cpg	160.20	J/mol×K	463.10	Joback Method
cpg	166.08	J/mol×K	490.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.68733e+01
Coeff. B	-4.00225e+03
Coeff. C	-4.89720e+01
Temperature range (K), min.	290.28
Temperature range (K), max.	395.13

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

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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