PROPANE, 1-CHLORO-3-ETHOXY-

Inchi: InChI=1S/C5H11ClO/c1-2-7-5-3-4-6/h2-5H2,1H3
InchiKey: AQVWVFMAJAIJFG-UHFFFAOYSA-N
Formula: C5H11ClO
SMILES: CCOCCCCl
Mol. weight [g/mol]: 122.59

Physical Properties

Property code	Value	Unit	Source
af	0.3740		Cheméo Relay (1.0)
gf	-125.71	kJ/mol	Joback Method
hf	-307.10	kJ/mol	Cheméo Relay (1.0)
hfus	14.09	kJ/mol	Joback Method
hvap	40.44	kJ/mol	Cheméo Relay (1.0)
ie	9.83	eV	Cheméo Relay (1.0)
log10ws	-0.83		Cheméo Relay (1.0)
logp	1.652		Crippen Method
mcvol	99.420	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	798.60		NIST Webbook
rinpol	794.80		NIST Webbook
tb	399.65 ± 3.00	K	NIST Webbook
tc	574.31	K	Cheméo Relay (1.0)
tf	180.93	K	Cheméo Relay (1.0)
vc	0.358	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.70	J/mol×K	373.65	Joback Method
cpg	181.40	J/mol×K	402.52	Joback Method
cpg	189.84	J/mol×K	431.40	Joback Method
cpg	198.02	J/mol×K	460.27	Joback Method
cpg	205.94	J/mol×K	489.15	Joback Method
cpg	213.61	J/mol×K	518.02	Joback Method

cpg	221.03	J/mol×K	546.90	Joback Method
dvisc	0.0033874	Pa×s	198.26	Joback Method
dvisc	0.0016880	Pa×s	227.49	Joback Method
dvisc	0.0009858	Pa×s	256.72	Joback Method
dvisc	0.0006426	Pa×s	285.95	Joback Method
dvisc	0.0004535	Pa×s	315.19	Joback Method
dvisc	0.0003395	Pa×s	344.42	Joback Method
dvisc	0.0002660	Pa×s	373.65	Joback Method

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36865380&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume