

PROPANE, 3-CHLORO-1,1-DIMETHOXY-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C5H11ClO2/c1-7-5(8-2)3-4-6/h5H,3-4H2,1-2H3

DXWRNRRBDAQWDB-UHFFFAOYSA-N

C5H11ClO2

COC(CCCl)OC

138.59

Physical Properties

Property code	Value	Unit	Source
hf	-438.35	kJ/mol	Cheméo Relay (1.0)
hfus	11.76	kJ/mol	Joback Method
hvap	46.07	kJ/mol	Cheméo Relay (1.0)
logp	1.234		Crippen Method
mcvol	105.290	ml/mol	McGowan Method
tb	424.87	K	Cheméo Relay (1.0)
tc	599.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.95	J/mol×K	395.63	Joback Method
cpg	202.76	J/mol×K	425.24	Joback Method
cpg	211.37	J/mol×K	454.86	Joback Method
cpg	219.76	J/mol×K	484.47	Joback Method
cpg	227.93	J/mol×K	514.09	Joback Method
cpg	235.87	J/mol×K	543.70	Joback Method
cpg	243.57	J/mol×K	573.32	Joback Method
dvisc	0.0040967	Pa×s	205.49	Joback Method
dvisc	0.0018358	Pa×s	237.18	Joback Method
dvisc	0.0009940	Pa×s	268.87	Joback Method
dvisc	0.0006125	Pa×s	300.56	Joback Method
dvisc	0.0004140	Pa×s	332.25	Joback Method
dvisc	0.0002995	Pa×s	363.94	Joback Method
dvisc	0.0002283	Pa×s	395.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.20	K	13.30	NIST Webbook
tbrp	324.20	K	2.50	NIST Webbook

Sources

Joback Method:	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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35502068&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

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