

cis-1-Propenyl tert-butyl ether

Inchi:	InChI=1S/C7H14O/c1-5-6-8-7(2,3)4/h5-6H,1-4H3/b6-5-
InchiKey:	XGCRQUBGQPXCPL-WAYWQWQTSA-N
Formula:	C7H14O
SMILES:	CC=COC(C)(C)C
Mol. weight [g/mol]:	114.19
CAS:	4188-71-0

Physical Properties

Property code	Value	Unit	Source
gf	-13.88	kJ/mol	Joback Method
hf	-211.56	kJ/mol	Joback Method
hfus	7.86	kJ/mol	Joback Method
hvap	32.25	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.335		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
tb	382.91	K	Joback Method
tc	567.42	K	Joback Method
tf	188.22	K	Joback Method
vc	0.414	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.24	J/molxK	382.91	Joback Method
cpg	218.07	J/molxK	413.66	Joback Method
cpg	230.26	J/molxK	444.41	Joback Method
cpg	241.85	J/molxK	475.16	Joback Method
cpg	252.86	J/molxK	505.92	Joback Method
cpg	263.31	J/molxK	536.67	Joback Method
cpg	273.23	J/molxK	567.42	Joback Method
dvisc	0.0070724	Paxs	188.22	Joback Method
dvisc	0.0025447	Paxs	220.67	Joback Method

dvisc	0.0011899	Paxs	253.12	Joback Method
dvisc	0.0006613	Paxs	285.56	Joback Method
dvisc	0.0004144	Paxs	318.01	Joback Method
dvisc	0.0002831	Paxs	350.46	Joback Method
dvisc	0.0002063	Paxs	382.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4188710&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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