

Tetrahydrofuran, 2-ethyl-5-methyl-

Inchi:	InChI=1S/C7H14O/c1-3-7-5-4-6(2)8-7/h6-7H,3-5H2,1-2H3
InchiKey:	UHMJZZUFLYFOBN-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CCC1CCC(C)O1
Mol. weight [g/mol]:	114.19
CAS:	931-39-5

Physical Properties

Property code	Value	Unit	Source
gf	-49.22	kJ/mol	Joback Method
hf	-279.67	kJ/mol	Joback Method
hfus	16.87	kJ/mol	Joback Method
hvap	35.63	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.964		Crippen Method
mvol	104.500	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
tb	390.65 ± 2.00	K	NIST Webbook
tb	390.65 ± 2.00	K	NIST Webbook
tc	591.40	K	Joback Method
tf	201.88	K	Joback Method
vc	0.389	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.71	J/molxK	397.12	Joback Method
cpg	219.81	J/molxK	429.50	Joback Method
cpg	234.23	J/molxK	461.88	Joback Method
cpg	248.01	J/molxK	494.26	Joback Method
cpg	261.14	J/molxK	526.64	Joback Method
cpg	273.66	J/molxK	559.02	Joback Method
cpg	285.56	J/molxK	591.40	Joback Method
dvisc	0.0027670	Paxs	201.88	Joback Method

dvisc	0.0015322	Paxs	234.42	Joback Method
dvisc	0.0009799	Paxs	266.96	Joback Method
dvisc	0.0006906	Paxs	299.50	Joback Method
dvisc	0.0005213	Paxs	332.04	Joback Method
dvisc	0.0004137	Paxs	364.58	Joback Method
dvisc	0.0003411	Paxs	397.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C931395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mcvol:	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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