

2-Isopropylidenetetrahydrofuran

Inchi:	InChI=1S/C7H12O/c1-6(2)7-4-3-5-8-7/h3-5H2,1-2H3
InchiKey:	UZXWDKGGOMPAEZ-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	CC(C)=C1CCCO1
Mol. weight [g/mol]:	112.17
CAS:	38614-14-1

Physical Properties

Property code	Value	Unit	Source
gf	3.11	kJ/mol	Joback Method
hf	-172.75	kJ/mol	Joback Method
hfus	13.74	kJ/mol	Joback Method
hvap	37.12	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	2.091		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
tb	412.98	K	Joback Method
tc	620.21	K	Joback Method
tf	206.76	K	Joback Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.81	J/mol×K	412.98	Joback Method
cpg	205.39	J/mol×K	447.52	Joback Method
cpg	218.22	J/mol×K	482.06	Joback Method
cpg	230.33	J/mol×K	516.59	Joback Method
cpg	241.74	J/mol×K	551.13	Joback Method
cpg	252.50	J/mol×K	585.67	Joback Method
cpg	262.64	J/mol×K	620.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38614141&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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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