

2,5-Dimethyl-3-(3-methylbutyl)-tetrahydrofuran

Inchi:	InChI=1S/C11H22O/c1-8(2)5-6-11-7-9(3)12-10(11)4/h8-11H,5-7H2,1-4H3
InchiKey:	RRMWFLAUEYCDIF-UHFFFAOYSA-N
Formula:	C11H22O
SMILES:	CC(C)CCC1CC(C)OC1C
Mol. weight [g/mol]:	170.29

Physical Properties

Property code	Value	Unit	Source
gf	-25.69	kJ/mol	Joback Method
hf	-387.85	kJ/mol	Joback Method
hfus	24.78	kJ/mol	Joback Method
hvap	43.84	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	3.236		Crippen Method
mvol	160.860	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1137.00		NIST Webbook
rinpol	1137.00		NIST Webbook
tb	483.53	K	Joback Method
tc	674.13	K	Joback Method
tf	227.72	K	Joback Method
vc	0.606	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.40	J/molxK	483.53	Joback Method
cpg	471.38	J/molxK	642.36	Joback Method
cpg	455.07	J/molxK	610.60	Joback Method
cpg	437.94	J/molxK	578.83	Joback Method
cpg	419.96	J/molxK	547.06	Joback Method
cpg	401.12	J/molxK	515.30	Joback Method
cpg	486.88	J/molxK	674.13	Joback Method
dvisc	0.0003266	Paxs	483.53	Joback Method

dvisc	0.0004010	Paxs	440.89	Joback Method
dvisc	0.0005145	Paxs	398.26	Joback Method
dvisc	0.0007008	Paxs	355.62	Joback Method
dvisc	0.0010384	Paxs	312.99	Joback Method
dvisc	0.0017416	Paxs	270.36	Joback Method
dvisc	0.0035453	Paxs	227.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R405699&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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