

trans-2-Methyl-5-ethyl-1,3-dioxane

Inchi:	InChI=1S/C7H14O2/c1-3-7-4-8-6(2)9-5-7/h6-7H,3-5H2,1-2H3/t6-,7-
InchiKey:	BXZQKMDNORUZLP-LJGSYFOKSA-N
Formula:	C7H14O2
SMILES:	CCC1COC(C)OC1
Mol. weight [g/mol]:	130.18
CAS:	25924-91-8

Physical Properties

Property code	Value	Unit	Source
chl	-4265.00 ± 10.00	kJ/mol	NIST Webbook
gf	-147.44	kJ/mol	Joback Method
hf	-417.83	kJ/mol	Joback Method
hfl	-491.00 ± 10.00	kJ/mol	NIST Webbook
hfus	22.75	kJ/mol	Joback Method
hvap	40.32	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.405		Crippen Method
mcvol	110.370	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
tb	428.34	K	Joback Method
tc	630.96	K	Joback Method
tf	224.93	K	Joback Method
vc	0.402	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.11	J/mol×K	428.34	Joback Method
cpg	305.59	J/mol×K	597.19	Joback Method
cpg	292.65	J/mol×K	563.42	Joback Method
cpg	279.04	J/mol×K	529.65	Joback Method
cpg	264.75	J/mol×K	495.88	Joback Method
cpg	249.78	J/mol×K	462.11	Joback Method
cpg	317.87	J/mol×K	630.96	Joback Method

dvisc	0.0003579	Paxs	428.34	Joback Method
dvisc	0.0004645	Paxs	394.44	Joback Method
dvisc	0.0006333	Paxs	360.54	Joback Method
dvisc	0.0009207	Paxs	326.63	Joback Method
dvisc	0.0014597	Paxs	292.73	Joback Method
dvisc	0.0026113	Paxs	258.83	Joback Method
dvisc	0.0055665	Paxs	224.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25924918&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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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