

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

Inchi:	InChI=1S/C9H18O2/c1-3-4-5-9-6-10-8(2)11-7-9/h8-9H,3-7H2,1-2H3/t8-,9-
InchiKey:	IJCIOLXHDMCLLI-KYZUINATSA-N
Formula:	C9H18O2
SMILES:	CCCCC1COC(C)OC1
Mol. weight [g/mol]:	158.24
CAS:	39087-22-4

Physical Properties

Property code	Value	Unit	Source
chl	-5566.00 ± 14.00	kJ/mol	NIST Webbook
gf	-130.60	kJ/mol	Joback Method
hf	-459.11	kJ/mol	Joback Method
hfl	-549.00 ± 14.00	kJ/mol	NIST Webbook
hfus	27.93	kJ/mol	Joback Method
hvap	44.77	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	2.186		Crippen Method
mcvol	138.550	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
tb	474.10	K	Joback Method
tc	671.99	K	Joback Method
tf	247.47	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.52	J/molxK	474.10	Joback Method
cpg	402.07	J/molxK	639.01	Joback Method
cpg	387.53	J/molxK	606.03	Joback Method
cpg	372.22	J/molxK	573.04	Joback Method
cpg	356.12	J/molxK	540.06	Joback Method
cpg	339.22	J/molxK	507.08	Joback Method
cpg	415.85	J/molxK	671.99	Joback Method

dvisc	0.0003243	Paxs	474.10	Joback Method
dvisc	0.0004255	Paxs	436.33	Joback Method
dvisc	0.0005879	Paxs	398.56	Joback Method
dvisc	0.0008692	Paxs	360.78	Joback Method
dvisc	0.0014079	Paxs	323.01	Joback Method
dvisc	0.0025914	Paxs	285.24	Joback Method
dvisc	0.0057462	Paxs	247.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39087224&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

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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