trans-2-Butyl-5-methyl-1,3-dioxane

Inchi: InChI=1S/C9H18O2/c1-3-4-5-9-10-6-8(2)7-11-9/h8-9H,3-7H2,1-2H3/t8-,9-
InchiKey: SJRRYRAMBIACCP-KYZUINATSA-N
Formula: C9H18O2
SMILES: CCCCC1OCC(C)CO1
Mol. weight [g/mol]: 158.24
CAS: 41824-29-7

Physical Properties

Property code	Value	Unit	Source
chl	-5499.00 ± 14.00	kJ/mol	NIST Webbook
gf	-130.60	kJ/mol	Joback Method
hf	-459.11	kJ/mol	Joback Method
hfl	-615.00 ± 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/mol×K	474.10	Joback Method
cpg	402.07	J/mol×K	639.01	Joback Method
cpg	387.53	J/mol×K	606.03	Joback Method
cpg	372.22	J/mol×K	573.04	Joback Method
cpg	356.12	J/mol×K	540.06	Joback Method
cpg	339.22	J/mol×K	507.08	Joback Method
cpg	415.85	J/mol×K	671.99	Joback Method

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

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41824297&Units=SI

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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