cis-2,4-Dimethyl-1,3-dioxane

Inchi: InChI=1S/C6H12O2/c1-5-3-4-7-6(2)8-5/h5-6H,3-4H2,1-2H3/t5-,6+/m0/s1
InchiKey: VREPYGYMOSZTKJ-NTSWFWBYSA-N
Formula: C6H12O2
SMILES: CC1CCOC(C)O1
Mol. weight [g/mol]: 116.16
CAS: 15042-59-8

Physical Properties

Property code	Value	Unit	Source
chl	-3610.80 ± 4.20	kJ/mol	NIST Webbook
chl	-3608.30 ± 1.40	kJ/mol	NIST Webbook
gf	-155.86	kJ/mol	Joback Method
hf	-425.20	kJ/mol	NIST Webbook
hf	-428.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-465.20 ± 4.20	kJ/mol	NIST Webbook
hfl	-468.00 ± 2.00	kJ/mol	NIST Webbook
hfus	20.16	kJ/mol	Joback Method
hvap	40.00 ± 1.00	kJ/mol	NIST Webbook
hvap	40.00	kJ/mol	NIST Webbook
log10ws	-1.12		Crippen Method
logp	1.158		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	390.65 ± 1.50	K	NIST Webbook
tc	610.20	K	Joback Method
tf	213.66	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.64	J/mol×K	405.46	Joback Method
cpg	208.06	J/mol×K	439.58	Joback Method
cpg	221.85	J/mol×K	473.71	Joback Method

cpg	235.02	J/mol×K	507.83	Joback Method
cpg	247.58	J/mol×K	541.95	Joback Method
cpg	259.54	J/mol×K	576.08	Joback Method
cpg	270.89	J/mol×K	610.20	Joback Method
dvisc	0.0052904	Pa×s	213.66	Joback Method
dvisc	0.0025382	Pa×s	245.63	Joback Method
dvisc	0.0014422	Pa×s	277.59	Joback Method
dvisc	0.0009210	Pa×s	309.56	Joback Method
dvisc	0.0006396	Pa×s	341.53	Joback Method
dvisc	0.0004728	Pa×s	373.49	Joback Method
dvisc	0.0003666	Pa×s	405.46	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=C15042598&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