1,3-Dioxolane, 4-methyl-2-propyl, cis

Other names: 1,3-Dioxolane, 4-methyl-2-propyl, trans
4-methyl-2-propyl-1,3-dioxolane
Inchi: InChI=1S/C7H14O2/c1-3-4-7-8-5-6(2)9-7/h6-7H,3-5H2,1-2H3
InchiKey: WRTYJFJOOTWPJP-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CCCC1OCC(C)O1
Mol. weight [g/mol]: 130.18
CAS: 4352-99-2

Physical Properties

Property code	Value	Unit	Source
gf	-135.34	kJ/mol	Joback Method
hf	-411.67	kJ/mol	Joback Method
hfus	24.85	kJ/mol	Joback Method
hvap	40.14	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.548		Crippen Method
mcvol	110.370	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	876.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	840.10		NIST Webbook
tb	424.07	K	Joback Method
tc	618.72	K	Joback Method
tf	228.45	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.21	J/mol×K	424.07	Joback Method
cpg	302.31	J/mol×K	586.28	Joback Method
cpg	290.14	J/mol×K	553.84	Joback Method
cpg	277.36	J/mol×K	521.39	Joback Method
cpg	263.96	J/mol×K	488.95	Joback Method
cpg	249.91	J/mol×K	456.51	Joback Method
cpg	313.87	J/mol×K	618.72	Joback Method
dvisc	0.0004061	Pa×s	424.07	Joback Method
dvisc	0.0005027	Pa×s	391.47	Joback Method
dvisc	0.0006469	Pa×s	358.86	Joback Method
dvisc	0.0008754	Pa×s	326.26	Joback Method
dvisc	0.0012670	Pa×s	293.66	Joback Method
dvisc	0.0020112	Pa×s	261.05	Joback Method
dvisc	0.0036427	Pa×s	228.45	Joback Method

Sources

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=C4352992&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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