1,3-Dioxane, 4-methyl-2-phenyl-

Other names: m-Dioxane, 4-methyl-2-phenyl-
2-Phenyl-4-methyl-1,3-dioxane
4-Methyl-2-phenyl-m-dioxane
4-Methyl-2-phenyl-1,3-dioxane
Inchi: InChI=1S/C11H14O2/c1-9-7-8-12-11(13-9)10-5-3-2-4-6-10/h2-6,9,11H,7-8H2,1H3
InchiKey: NJDSRMVYAFOBIZ-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CC1CCOC(c2ccccc2)O1
Mol. weight [g/mol]: 178.23
CAS: 774-44-7

Physical Properties

Property code	Value	Unit	Source
gf	-1.35	kJ/mol	Joback Method
hf	-263.86	kJ/mol	Joback Method
hfus	27.15	kJ/mol	Joback Method
hvap	51.50	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.511		Crippen Method
mcvol	142.970	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
tb	546.54	K	Joback Method
tc	786.46	K	Joback Method
tf	296.43	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.56	J/mol×K	546.54	Joback Method
cpg	369.78	J/mol×K	586.53	Joback Method
cpg	387.69	J/mol×K	626.51	Joback Method
cpg	404.33	J/mol×K	666.50	Joback Method
cpg	419.73	J/mol×K	706.49	Joback Method

cpg	433.95	J/mol×K	746.47	Joback Method
cpg	447.01	J/mol×K	786.46	Joback Method
dvisc	0.0038201	Pa×s	296.43	Joback Method
dvisc	0.0018759	Pa×s	338.12	Joback Method
dvisc	0.0010769	Pa×s	379.80	Joback Method
dvisc	0.0006899	Pa×s	421.49	Joback Method
dvisc	0.0004789	Pa×s	463.17	Joback Method
dvisc	0.0003530	Pa×s	504.85	Joback Method
dvisc	0.0002727	Pa×s	546.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C774447&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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