1,3-Dioxane, 2-phenyl-

Other names:	m-Dioxane, 2-phenyl-
	2-Phenyl-m-dioxane
	2-Phenyl-1,3-dioxan
	2-Phenyl-1,3-dioxane
Inchi:	InChI=1S/C10H12O2/c1-2-5-9(6-3-1)10-11-7-4-8-12-10/h1-3,5-6,10H,4,7-8H2
InchiKey:	LNEMDIUSUQPKIP-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	c1ccc(C2OCCCO2)cc1
Mol. weight [g/mol]:	164.20
CAS:	772-01-0

Physical Properties

Property code	Value	Unit	Source
gf	-2.06	kJ/mol	Joback Method
hf	-222.88	kJ/mol	Joback Method
hfus	23.49	kJ/mol	Joback Method
hvap	49.58	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.122		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	1344.00		NIST Webbook
tb	528.33	K	Joback Method
tc	773.22	K	Joback Method
tf	321.65 ± 1.50	K	NIST Webbook
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.25	J/mol×K	528.33	Joback Method
cpg	379.73	J/mol×K	732.40	Joback Method
cpg	366.63	J/mol×K	691.59	Joback Method
cpg	352.38	J/mol×K	650.77	Joback Method

cpg	336.94	J/mol×K	609.96	Joback Method
cpg	320.24	J/mol×K	569.14	Joback Method
cpg	391.73	J/mol×K	773.22	Joback Method
dvisc	0.0002690	Pa×s	528.33	Joback Method
dvisc	0.0003586	Pa×s	488.51	Joback Method
dvisc	0.0005031	Pa×s	448.69	Joback Method
dvisc	0.0007539	Pa×s	408.86	Joback Method
dvisc	0.0012328	Pa×s	369.04	Joback Method
dvisc	0.0022707	Pa×s	329.22	Joback Method
dvisc	0.0049478	Pa×s	289.40	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=C772010&Units=SI

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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