

1,3-Dioxolane, 2-(phenylmethyl)-

Other names:	1,3-Dioxolane, 2-benzyl- Phenylacetaldehyde ethylene acetal Phenylacetaldehyde glycol acetal 2-Benzyl-1,3-dioxolane Phenylacetaldehyde ethylene glycol acetal 2-Benzylidioxolan
Inchi:	InChI=1S/C10H12O2/c1-2-4-9(5-3-1)8-10-11-6-7-12-10/h1-5,10H,6-8H2
InchiKey:	SSZACLYPEFCREM-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	c1ccc(CC2OCCO2)cc1
Mol. weight [g/mol]:	164.20
CAS:	101-49-5

Physical Properties

Property code	Value	Unit	Source
gf	10.04	kJ/mol	Joback Method
hf	-216.72	kJ/mol	Joback Method
hfus	25.59	kJ/mol	Joback Method
hvap	49.41	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.602		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpol	1276.90		NIST Webbook
rinpol	1276.90		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1940.00		NIST Webbook
tb	524.06	K	Joback Method
tc	759.82	K	Joback Method
tf	292.92	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.00	J/mol×K	524.06	Joback Method
cpg	375.17	J/mol×K	720.53	Joback Method
cpg	362.71	J/mol×K	681.23	Joback Method
cpg	349.22	J/mol×K	641.94	Joback Method
cpg	334.64	J/mol×K	602.65	Joback Method
cpg	318.92	J/mol×K	563.35	Joback Method
cpg	386.66	J/mol×K	759.82	Joback Method
dvisc	0.0003354	Pa×s	524.06	Joback Method
dvisc	0.0004306	Pa×s	485.54	Joback Method
dvisc	0.0005771	Pa×s	447.01	Joback Method
dvisc	0.0008174	Pa×s	408.49	Joback Method
dvisc	0.0012448	Pa×s	369.97	Joback Method
dvisc	0.0020905	Pa×s	331.44	Joback Method
dvisc	0.0040235	Pa×s	292.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.70	K	1.60	NIST Webbook

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=C101495&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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