

1,3-Dioxolane, 2-(4-methoxyphenyl)-4-methyl, # 1

Inchi:	InChI=1S/C11H14O3/c1-8-7-13-11(14-8)9-3-5-10(12-2)6-4-9/h3-6,8,11H,7H2,1-2H3
InchiKey:	DTACWEXJFYOAKS-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	COc1ccc(C2OCC(C)O2)cc1
Mol. weight [g/mol]:	194.23

Physical Properties

Property code	Value	Unit	Source
gf	-103.88	kJ/mol	Joback Method
hf	-401.39	kJ/mol	Joback Method
hfus	30.05	kJ/mol	Joback Method
hvap	54.40	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.129		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
rinpol	1508.00		NIST Webbook
rinpol	1508.00		NIST Webbook
ripol	2231.00		NIST Webbook
ripol	2231.00		NIST Webbook
tb	569.67	K	Joback Method
tc	798.91	K	Joback Method
tf	334.70	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.86	J/molxK	569.67	Joback Method
cpg	393.15	J/molxK	607.88	Joback Method
cpg	409.37	J/molxK	646.08	Joback Method
cpg	424.56	J/molxK	684.29	Joback Method
cpg	438.72	J/molxK	722.50	Joback Method
cpg	451.88	J/molxK	760.70	Joback Method

cpg	464.06	J/molxK	798.91	Joback Method
dvisc	0.0019113	Paxs	334.70	Joback Method
dvisc	0.0011703	Paxs	373.86	Joback Method
dvisc	0.0007864	Paxs	413.02	Joback Method
dvisc	0.0005661	Paxs	452.19	Joback Method
dvisc	0.0004295	Paxs	491.35	Joback Method
dvisc	0.0003394	Paxs	530.51	Joback Method
dvisc	0.0002770	Paxs	569.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R409171&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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