

4-(4,5-Dimethyl-1,3-dioxolan-2-yl)-2-methoxyphen

Inchi:	InChI=1S/C12H16O4/c1-7-8(2)16-12(15-7)9-4-5-10(13)11(6-9)14-3/h4-8,12-13H,1-3H3
InchiKey:	JZJHVHUFPUYAJF-UHFFFAOYSA-N
Formula:	C12H16O4
SMILES:	COc1cc(C2OC(C)C(C)O2)ccc1O
Mol. weight [g/mol]:	224.25
CAS:	63253-24-7

Physical Properties

Property code	Value	Unit	Source
gf	-257.79	kJ/mol	Joback Method
hf	-619.68	kJ/mol	Joback Method
hfus	39.49	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.223		Crippen Method
mcvol	168.800	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	1750.90		NIST Webbook
rinpol	1750.90		NIST Webbook
tb	668.50	K	Joback Method
tc	902.41	K	Joback Method
tf	453.45	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.45	J/molxK	668.50	Joback Method
cpg	556.02	J/molxK	863.42	Joback Method
cpg	543.60	J/molxK	824.44	Joback Method
cpg	530.30	J/molxK	785.45	Joback Method
cpg	516.05	J/molxK	746.47	Joback Method
cpg	500.78	J/molxK	707.48	Joback Method
cpg	567.61	J/molxK	902.41	Joback Method

dvisc	0.0000338	Paxs	668.50	Joback Method
dvisc	0.0000471	Paxs	632.66	Joback Method
dvisc	0.0000684	Paxs	596.82	Joback Method
dvisc	0.0001042	Paxs	560.98	Joback Method
dvisc	0.0001680	Paxs	525.13	Joback Method
dvisc	0.0002905	Paxs	489.29	Joback Method
dvisc	0.0005477	Paxs	453.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63253247&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

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
mvol:	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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