iso-Butyl aldehyde-1-phenyl-1,2-ethanediol acetal

Other names: 1,3-Dioxolane, 2-(1-methylethyl)-4-phenyl
1,3-Dioxolane, 2-isopropyl-4-phenyl
Inchi: InChI=1S/C12H16O2/c1-9(2)12-13-8-11(14-12)10-6-4-3-5-7-10/h3-7,9,11-12H,8H2,1-2H
InchiKey: LYTZYXJGLNHQAS-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: CC(C)C1OCC(c2ccccc2)O1
Mol. weight [g/mol]: 192.25
CAS: 55668-34-3

Physical Properties

Property code	Value	Unit	Source
gf	16.73	kJ/mol	Joback Method
hf	-283.62	kJ/mol	Joback Method
hfus	28.32	kJ/mol	Joback Method
hvap	53.16	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.757		Crippen Method
mcvol	157.060	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1384.00		NIST Webbook
rinpol	1384.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1900.00		NIST Webbook
tb	564.71	K	Joback Method
tc	796.68	K	Joback Method
tf	296.22	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.67	J/mol×K	564.71	Joback Method
cpg	417.91	J/mol×K	603.37	Joback Method
cpg	435.85	J/mol×K	642.03	Joback Method

cpg	452.53	J/mol×K	680.70	Joback Method
cpg	468.03	J/mol×K	719.36	Joback Method
cpg	482.37	J/mol×K	758.02	Joback Method
cpg	495.63	J/mol×K	796.68	Joback Method
dvisc	0.0041016	Pa×s	296.22	Joback Method
dvisc	0.0019934	Pa×s	340.97	Joback Method
dvisc	0.0011454	Pa×s	385.72	Joback Method
dvisc	0.0007385	Pa×s	430.47	Joback Method
dvisc	0.0005172	Pa×s	475.21	Joback Method
dvisc	0.0003851	Pa×s	519.96	Joback Method
dvisc	0.0003004	Pa×s	564.71	Joback Method

Sources

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=C55668343&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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