

Methyl n-hexyl ketone-1-phenyl-1,2-ethanediol ketal 1

Other names:	1,3-Dioxolane, 2-methyl-2-hexyl-4-phenyl, # 1
Inchi:	InChI=1S/C16H24O2/c1-3-4-5-9-12-16(2)17-13-15(18-16)14-10-7-6-8-11-14/h6-8,10-11,
InchiKey:	ZYMAQLGBEVTHJC-UHFFFAOYSA-N
Formula:	C16H24O2
SMILES:	CCCCCCC1(C)OCC(c2ccccc2)O1
Mol. weight [g/mol]:	248.36

Physical Properties

Property code	Value	Unit	Source
gf	47.36	kJ/mol	Joback Method
hf	-345.66	kJ/mol	Joback Method
hfus	35.90	kJ/mol	Joback Method
hvap	61.30	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.461		Crippen Method
mcvol	213.420	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	1739.00		NIST Webbook
rinpol	1739.00		NIST Webbook
ripol	2224.00		NIST Webbook
ripol	2224.00		NIST Webbook
tb	656.91	K	Joback Method
tc	875.90	K	Joback Method
tf	380.20	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.73	J/mol×K	656.91	Joback Method
cpg	623.84	J/mol×K	693.41	Joback Method
cpg	642.84	J/mol×K	729.91	Joback Method
cpg	660.85	J/mol×K	766.40	Joback Method
cpg	678.03	J/mol×K	802.90	Joback Method

cpg	694.52	J/mol×K	839.40	Joback Method
cpg	710.47	J/mol×K	875.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U285397&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
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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