

2-ACETYLPHENOL BENZYL ETHER

Other names:	2-Acetylphenol benzyl ether 2-Benzyloxyacetophenone
Inchi:	InChI=1S/C15H14O2/c1-12(16)14-9-5-6-10-15(14)17-11-13-7-3-2-4-8-13/h2-10H,11H2,1
InchiKey:	ZJABPUSDYOXUKS-UHFFFAOYSA-N
Formula:	C15H14O2
SMILES:	CC(=O)c1ccccc1OCc1ccccc1
Mol. weight [g/mol]:	226.28

Physical Properties

Property code	Value	Unit	Source
hf	-134.76	kJ/mol	Cheméo Relay (1.0)
hfus	25.09	kJ/mol	Joback Method
hvap	84.50	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-3.57		Cheméo Relay (1.0)
logp	3.468		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
tb	601.63	K	Cheméo Relay (1.0)
tf	315.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.84	J/mol×K	677.23	Joback Method
cpg	481.42	J/mol×K	716.99	Joback Method
cpg	495.81	J/mol×K	756.74	Joback Method
cpg	509.05	J/mol×K	796.50	Joback Method
cpg	521.19	J/mol×K	836.25	Joback Method
cpg	532.27	J/mol×K	876.01	Joback Method
cpg	542.35	J/mol×K	915.77	Joback Method
dvisc	0.0012300	Pa×s	396.33	Joback Method
dvisc	0.0007015	Pa×s	443.15	Joback Method
dvisc	0.0004454	Pa×s	489.96	Joback Method
dvisc	0.0003061	Pa×s	536.78	Joback Method

dvisc	0.0002234	Pa×s	583.60	Joback Method
dvisc	0.0001709	Pa×s	630.41	Joback Method
dvisc	0.0001356	Pa×s	677.23	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31165670&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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