

Ethanal, ethyl phenylethyl acetal

Inchi:	InChI=1S/C12H18O2/c1-3-13-11(2)14-10-9-12-7-5-4-6-8-12/h4-8,11H,3,9-10H2,1-2H3
InchiKey:	QQDGMPOYFGNLMU-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	CCOC(C)OCCc1ccccc1
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
gf	-49.87	kJ/mol	Joback Method
hf	-324.20	kJ/mol	Joback Method
hfus	19.73	kJ/mol	Joback Method
hvap	49.01	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.628		Crippen Method
mvol	167.920	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
ripol	1332.00		NIST Webbook
ripol	1770.00		NIST Webbook
tb	545.04	K	Joback Method
tc	745.23	K	Joback Method
tf	280.88	K	Joback Method
vc	0.629	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.63	J/molxK	545.04	Joback Method
cpg	472.98	J/molxK	711.87	Joback Method
cpg	459.67	J/molxK	678.50	Joback Method
cpg	445.59	J/molxK	645.14	Joback Method
cpg	430.74	J/molxK	611.77	Joback Method
cpg	415.09	J/molxK	578.41	Joback Method
cpg	485.53	J/molxK	745.23	Joback Method
dvisc	0.0001324	Paxs	545.04	Joback Method

dvisc	0.0001758	Paxs	501.01	Joback Method
dvisc	0.0002464	Paxs	456.99	Joback Method
dvisc	0.0003711	Paxs	412.96	Joback Method
dvisc	0.0006164	Paxs	368.93	Joback Method
dvisc	0.0011747	Paxs	324.91	Joback Method
dvisc	0.0027402	Paxs	280.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R409780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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