

Benzeneethanol, «alpha»-ethyl-

Other names:	Phenethyl alcohol, «alpha»-ethyl- Benzyl ethyl carbinol 2-Butanol, 1-phenyl- «alpha»-Ethylphenethyl alcohol 1-Phenyl-2-butanol «alpha»-Ethylbenzeneethanol 1-phenylbutan-2-ol
Inchi:	InChI=1S/C10H14O/c1-2-10(11)8-9-6-4-3-5-7-9/h3-7,10-11H,2,8H2,1H3
InchiKey:	LYUPJHVGLFETDG-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CCC(O)Cc1ccccc1
Mol. weight [g/mol]:	150.22
CAS:	701-70-2

Physical Properties

Property code	Value	Unit	Source
gf	6.47	kJ/mol	Joback Method
hf	-170.71	kJ/mol	Joback Method
hfus	16.26	kJ/mol	Joback Method
hvap	56.42	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.000		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	1232.00		NIST Webbook
rinpol	1222.00		NIST Webbook
ripol	1882.00		NIST Webbook
tb	546.62	K	Joback Method
tc	743.00	K	Joback Method
tf	274.70	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.06	J/mol×K	546.62	Joback Method
cpg	369.24	J/mol×K	710.27	Joback Method
cpg	359.13	J/mol×K	677.54	Joback Method
cpg	348.39	J/mol×K	644.81	Joback Method
cpg	336.98	J/mol×K	612.08	Joback Method
cpg	324.88	J/mol×K	579.35	Joback Method
cpg	378.75	J/mol×K	743.00	Joback Method
dvisc	0.0001002	Pa×s	546.62	Joback Method
dvisc	0.0001658	Pa×s	501.30	Joback Method
dvisc	0.0003030	Pa×s	455.98	Joback Method
dvisc	0.0006329	Pa×s	410.66	Joback Method
dvisc	0.0015868	Pa×s	365.34	Joback Method
dvisc	0.0051616	Pa×s	320.02	Joback Method
dvisc	0.0247773	Pa×s	274.70	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.70	K	3.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C701702&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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