

Benzenemethanol, «alpha»-2-propenyl-

Other names:	1-Phenyl-but-3-en-1-ol «alpha»-2-Propenyl-benzenmethanol
Inchi:	InChI=1S/C10H12O/c1-2-6-10(11)9-7-4-3-5-8-9/h2-5,7-8,10-11H,1,6H2
InchiKey:	RGKVZBXSJFAZRE-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	C=CCC(O)c1ccccc1
Mol. weight [g/mol]:	148.20
CAS:	936-58-3

Physical Properties

Property code	Value	Unit	Source
gf	94.31	kJ/mol	Joback Method
hf	-45.28	kJ/mol	Joback Method
hfus	14.98	kJ/mol	Joback Method
hvap	55.75	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.296		Crippen Method
mvol	129.570	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
ripol	1869.00		NIST Webbook
ripol	1869.00		NIST Webbook
tb	543.30	K	Joback Method
tc	743.63	K	Joback Method
tf	272.94	K	Joback Method
vc	0.481	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.88	J/mol×K	543.30	Joback Method
cpg	305.05	J/mol×K	576.69	Joback Method
cpg	316.48	J/mol×K	610.08	Joback Method
cpg	327.21	J/mol×K	643.46	Joback Method
cpg	337.28	J/mol×K	676.85	Joback Method

cpg	346.71	J/mol×K	710.24	Joback Method
cpg	355.55	J/mol×K	743.63	Joback Method
dvisc	0.0237151	Paxs	272.94	Joback Method
dvisc	0.0050542	Paxs	318.00	Joback Method
dvisc	0.0015810	Paxs	363.06	Joback Method
dvisc	0.0006392	Paxs	408.12	Joback Method
dvisc	0.0003095	Paxs	453.18	Joback Method
dvisc	0.0001708	Paxs	498.24	Joback Method
dvisc	0.0001041	Paxs	543.30	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=C936583&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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