

Benzenemethanol, «alpha»-propyl-

Other names:	alpha-n-Propyl benzyl alcohol «alpha»-Propylbenzyl alcohol 1-Butanol, 1-phenyl 1-Phenylbutan-1-ol
Inchi:	InChI=1S/C10H14O/c1-2-6-10(11)9-7-4-3-5-8-9/h3-5,7-8,10-11H,2,6H2,1H3
InchiKey:	HQRWWHIETAKIMO-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CCCC(O)c1ccccc1
Mol. weight [g/mol]:	150.22
CAS:	614-14-2

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	-2.83		Crippen Method
logp	2.520		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	1310.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1220.30		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1955.00		NIST Webbook
tb	506.15 ± 2.00	K	NIST Webbook
tc	743.00	K	Joback Method
tf	274.70	K	Joback Method
vc	0.500	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C614142&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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