

Benzenemethanol, 4-(1,1-dimethylethyl)-

Other names:	p-tert-Butylbenzyl alcohol 4-tert-Butylbenzyl alcohol 4(t-Butyl)benzylalcohol
Inchi:	InChI=1S/C11H16O/c1-11(2,3)10-6-4-9(8-12)5-7-10/h4-7,12H,8H2,1-3H3
InchiKey:	FVEINXLJOJPHLH-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	CC(C)(C)c1ccc(CO)cc1
Mol. weight [g/mol]:	164.24
CAS:	877-65-6

Physical Properties

Property code	Value	Unit	Source
gf	10.54	kJ/mol	Joback Method
hf	-206.29	kJ/mol	Joback Method
hfus	14.57	kJ/mol	Joback Method
hvap	58.40	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.476		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1336.00		NIST Webbook
tb	571.69	K	Joback Method
tc	773.69	K	Joback Method
tf	315.91	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.53	J/molxK	571.69	Joback Method
cpg	375.27	J/molxK	605.36	Joback Method
cpg	388.16	J/molxK	639.02	Joback Method
cpg	400.25	J/molxK	672.69	Joback Method
cpg	411.58	J/molxK	706.36	Joback Method

cpg	422.21	J/molxK	740.03	Joback Method
cpg	432.17	J/molxK	773.69	Joback Method
dvisc	0.0083872	Paxs	315.91	Joback Method
dvisc	0.0024328	Paxs	358.54	Joback Method
dvisc	0.0009179	Paxs	401.17	Joback Method
dvisc	0.0004177	Paxs	443.80	Joback Method
dvisc	0.0002182	Paxs	486.43	Joback Method
dvisc	0.0001265	Paxs	529.06	Joback Method
dvisc	0.0000796	Paxs	571.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	2.70	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C877656&Units=SI

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
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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