

Benzenemethanol, 2,4,5-trimethyl-

Other names:	Benzyl alcohol, 2,4,5-trimethyl- «alpha»-Durenol Pseudocumene-5-methylol 2,4,5-Trimethylbenzyl alcohol 2,4,5-Trimethyl-benzenemethanol
Inchi:	InChI=1S/C10H14O/c1-7-4-9(3)10(6-11)5-8(7)2/h4-5,11H,6H2,1-3H3
InchiKey:	GHDQBJLOOLNHCJ-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	<chem>Cc1cc(C)c(CO)cc1C</chem>
Mol. weight [g/mol]:	150.22
CAS:	4393-05-9

Physical Properties

Property code	Value	Unit	Source
gf	-19.98	kJ/mol	Joback Method
hf	-199.84	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Joback Method
hvap	58.80	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.104		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	562.00	K	Joback Method
tc	757.46	K	Joback Method
tf	327.26	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.51	J/molxK	562.00	Joback Method
cpg	322.19	J/molxK	594.58	Joback Method
cpg	333.33	J/molxK	627.15	Joback Method
cpg	343.94	J/molxK	659.73	Joback Method

cpg	354.02	J/mol×K	692.31	Joback Method
cpg	363.60	J/mol×K	724.89	Joback Method
cpg	372.69	J/mol×K	757.46	Joback Method
dvisc	0.0035304	Paxs	327.26	Joback Method
dvisc	0.0013925	Paxs	366.38	Joback Method
dvisc	0.0006572	Paxs	405.51	Joback Method
dvisc	0.0003540	Paxs	444.63	Joback Method
dvisc	0.0002108	Paxs	483.75	Joback Method
dvisc	0.0001356	Paxs	522.88	Joback Method
dvisc	0.0000928	Paxs	562.00	Joback Method

Sources

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=C4393059&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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