p-Chloro-«alpha»,«alpha»-dimethylphenethyl alcohol

Other names: Benzeneethanol, 4-chloro-«alpha»,«alpha»-dimethyl-
Benzenethanol, 4-chloro-«alpha»,«alpha»-dimethyl-
4-chloro-«alpha»,«alpha»-dimethylphenethylic alcohol

Inchi: InChI=1S/C10H13ClO/c1-10(2,12)7-8-3-5-9(11)6-4-8/h3-6,12H,7H2,1-2H3

InchiKey: WAAJRPRSQXYYAA-UHFFFAOYSA-N

Formula: C10H13ClO

SMILES: CC(C)(O)Cc1ccc(Cl)cc1

Mol. weight [g/mol]: 184.66

CAS: 5468-97-3

Physical Properties

Property code	Value	Unit	Source
gf	-9.81	kJ/mol	Joback Method
hf	-201.39	kJ/mol	Joback Method
hfus	16.18	kJ/mol	Joback Method
hvap	60.56	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.653		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	586.24	K	Joback Method
tc	795.56	K	Joback Method
tf	334.56	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.76	J/mol×K	586.24	Joback Method
cpg	393.48	J/mol×K	760.68	Joback Method
cpg	384.37	J/mol×K	725.79	Joback Method
cpg	374.59	J/mol×K	690.90	Joback Method
cpg	364.10	J/mol×K	656.01	Joback Method
cpg	352.84	J/mol×K	621.13	Joback Method

cpg	401.98	J/mol×K	795.56	Joback Method
dvisc	0.0000805	Pa×s	586.24	Joback Method
dvisc	0.0001253	Pa×s	544.29	Joback Method
dvisc	0.0002100	Pa×s	502.35	Joback Method
dvisc	0.0003866	Pa×s	460.40	Joback Method
dvisc	0.0008044	Pa×s	418.45	Joback Method
dvisc	0.0019708	Pa×s	376.51	Joback Method
dvisc	0.0060450	Pa×s	334.56	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5468973&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

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