2,3,4,5,6-Pentafluorobenzyl alcohol

Other names:	Pentafluorobenzyl alcohol Benzenemethanol, 2,3,4,5,6-pentafluoro- Benzyl alcohol, 2,3,4,5,6-pentafluoro- (Hydroxymethyl)pentafluorobenzene (Pentafluorophenyl)methanol 2,3,4,5,6-pentafluorobenzylic alcohol
Inchi:	InChI=1S/C7H3F5O/c8-3-2(1-13)4(9)6(11)7(12)5(3)10/h13H,1H2
InchiKey:	PGJYYCIOYBZTPU-UHFFFAOYSA-N
Formula:	C7H3F5O
SMILES:	OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	198.09
CAS:	440-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-1038.55	kJ/mol	Joback Method
hf	-1141.41	kJ/mol	Joback Method
hfus	25.47	kJ/mol	Joback Method
hvap	49.36	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	1.874		Crippen Method
mcvol	100.450	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	454.00 ± 1.00	K	NIST Webbook
tb	454.20	K	NIST Webbook
tc	661.64	K	Joback Method
tf	321.44	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.50	J/mol×K	499.67	Joback Method
cpg	228.55	J/mol×K	526.66	Joback Method

cpg	234.39	J/mol×K	553.66	Joback Method
cpg	240.01	J/mol×K	580.65	Joback Method
cpg	245.42	J/mol×K	607.65	Joback Method
cpg	250.62	J/mol×K	634.64	Joback Method
cpg	255.61	J/mol×K	661.64	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.70	K	8.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C440608&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
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume