3,3,4,4,4-pentafluorobutan-2-ol

Other names: Pentafluorobutanol-2
Inchi: InChI=1S/C4H5F5O/c1-2(10)3(5,6)4(7,8)9/h2,10H,1H3
InchiKey: BUGIAHXXBFVPGW-UHFFFAOYSA-N
Formula: C4H5F5O
SMILES: CC(O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 164.07
CAS: 374-40-3

Physical Properties

Property code	Value	Unit	Source
gf	-1124.83	kJ/mol	Joback Method
hf	-1281.45	kJ/mol	Joback Method
hfus	7.25	kJ/mol	Joback Method
hvap	34.11	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.565		Crippen Method
mcvol	81.940	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	357.00 ± 1.00	K	NIST Webbook
tc	516.48	K	Joback Method
tf	188.45	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.56	J/mol×K	372.55	Joback Method
cpg	186.44	J/mol×K	396.54	Joback Method
cpg	193.87	J/mol×K	420.53	Joback Method
cpg	200.86	J/mol×K	444.51	Joback Method
cpg	207.44	J/mol×K	468.50	Joback Method
cpg	213.61	J/mol×K	492.49	Joback Method
cpg	219.41	J/mol×K	516.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C374403&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume