

2-Butanol, 3,3,4,4-tetrafluoro-2-methyl-

Other names:	2-Methyl-3,3,4,4-tetrafluoro-2-butanol 2,2,3,3-Tetrafluoro-1,1-dimethylpropanol 2-Butanol, 2-methyl-3,3,4,4-tetrafluoro- 3,3,4,4-tetrafluoro-2-methylbutan-2-ol
Inchi:	InChI=1S/C5H8F4O/c1-4(2,10)5(8,9)3(6)7/h3,10H,1-2H3
InchiKey:	NCMPMCXQKBZXGI-UHFFFAOYSA-N
Formula:	C5H8F4O
SMILES:	CC(C)(O)C(F)(F)C(F)F
Mol. weight [g/mol]:	160.11
CAS:	29553-26-2

Physical Properties

Property code	Value	Unit	Source
gf	-921.60	kJ/mol	Joback Method
hf	-1105.98	kJ/mol	Joback Method
hfus	6.76	kJ/mol	Joback Method
hvap	37.16	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.658		Crippen Method
mcvol	94.260	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	396.16	K	Joback Method
tc	547.81	K	Joback Method
tf	199.13	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.71	J/molxK	396.16	Joback Method
cpg	215.93	J/molxK	421.44	Joback Method
cpg	224.63	J/molxK	446.71	Joback Method
cpg	232.83	J/molxK	471.99	Joback Method
cpg	240.56	J/molxK	497.26	Joback Method

cpg	247.82	J/mol×K	522.54	Joback Method
cpg	254.65	J/mol×K	547.81	Joback Method

Sources

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=C29553262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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