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

Inchi: InChI=1S/C4H6F4O/c1-2(9)4(7,8)3(5)6/h2-3,9H,1H3
InchiKey: UPMGUZUMWYWMKI-UHFFFAOYSA-N
Formula: C4H6F4O
SMILES: CC(O)C(F)(F)C(F)F
Mol. weight [g/mol]: 146.08
CAS: 17425-25-1

Physical Properties

Property code	Value	Unit	Source
gf	-935.30	kJ/mol	Joback Method
hf	-1081.87	kJ/mol	Joback Method
hfus	8.06	kJ/mol	Joback Method
hvap	35.84	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.268		Crippen Method
mcvol	80.170	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	376.07	K	Joback Method
tc	521.99	K	Joback Method
tf	170.44	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.93	J/mol×K	376.07	Joback Method
cpg	176.28	J/mol×K	400.39	Joback Method
cpg	183.28	J/mol×K	424.71	Joback Method
cpg	189.93	J/mol×K	449.03	Joback Method
cpg	196.25	J/mol×K	473.35	Joback Method
cpg	202.26	J/mol×K	497.67	Joback Method
cpg	207.95	J/mol×K	521.99	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=C17425251&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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