4,4,4-Trifluorobutanol

Other names: 1-Butanol, 4,4,4-trifluoro-
Inchi: InChI=1S/C4H7F3O/c5-4(6,7)2-1-3-8/h8H,1-3H2
InchiKey: VKRFUGHXKNNIJO-UHFFFAOYSA-N
Formula: C4H7F3O
SMILES: OCCCC(F)(F)F
Mol. weight [g/mol]: 128.09
CAS: 461-18-7

Physical Properties

Property code	Value	Unit	Source
gf	-735.61	kJ/mol	Joback Method
hf	-875.20	kJ/mol	Joback Method
hfus	12.03	kJ/mol	Joback Method
hvap	37.43	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.321		Crippen Method
mcvol	78.400	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	377.68	K	Joback Method
tc	524.81	K	Joback Method
tf	199.85	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.78	J/mol×K	377.68	Joback Method
cpg	167.98	J/mol×K	402.20	Joback Method
cpg	174.83	J/mol×K	426.72	Joback Method
cpg	181.36	J/mol×K	451.25	Joback Method
cpg	187.57	J/mol×K	475.77	Joback Method
cpg	193.47	J/mol×K	500.29	Joback Method
cpg	199.09	J/mol×K	524.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C461187&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