3,3,3-Trifluoro-1-propanol

Other names: 3,3,3-Trifluoropropan-1-ol
Inchi: InChI=1S/C3H5F3O/c4-3(5,6)1-2-7/h7H,1-2H2
InchiKey: HDBGBTNNPRCVND-UHFFFAOYSA-N
Formula: C3H5F3O
SMILES: OCCC(F)(F)F
Mol. weight [g/mol]: 114.07
CAS: 2240-88-2

Physical Properties

Property code	Value	Unit	Source
gf	-744.03	kJ/mol	Joback Method
hf	-854.56	kJ/mol	Joback Method
hfus	9.44	kJ/mol	Joback Method
hvap	35.20	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	0.931		Crippen Method
mcvol	64.310	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
tb	354.80	K	Joback Method
tc	501.48	K	Joback Method
tf	188.58	K	Joback Method
vc	0.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.27	J/mol×K	354.80	Joback Method
cpg	133.31	J/mol×K	379.25	Joback Method
cpg	139.04	J/mol×K	403.69	Joback Method
cpg	144.49	J/mol×K	428.14	Joback Method
cpg	149.66	J/mol×K	452.58	Joback Method
cpg	154.56	J/mol×K	477.03	Joback Method
cpg	159.20	J/mol×K	501.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2240882&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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