2,2,2-trifluoro-N-(hydroxymethyl)acetamide

Inchi: InChI=1S/C3H4F3NO2/c4-3(5,6)2(9)7-1-8/h8H,1H2,(H,7,9)
InchiKey: URUWXKFAEKTWKG-UHFFFAOYSA-N
Formula: C3H4F3NO2
SMILES: O=C(NCO)C(F)(F)F
Mol. weight [g/mol]: 143.06
CAS: 50667-69-1

Physical Properties

Property code	Value	Unit	Source
gf	-783.56	kJ/mol	Joback Method
hf	-913.67	kJ/mol	Joback Method
hfus	16.14	kJ/mol	Joback Method
hvap	48.39	kJ/mol	Joback Method
log10ws	-0.46		Crippen Method
logp	-0.385		Crippen Method
mcvol	75.860	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
tb	458.84	K	Joback Method
tc	622.34	K	Joback Method
tf	291.17	K	Joback Method
vc	0.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.05	J/mol×K	458.84	Joback Method
cpg	178.99	J/mol×K	486.09	Joback Method
cpg	184.57	J/mol×K	513.34	Joback Method
cpg	189.82	J/mol×K	540.59	Joback Method
cpg	194.74	J/mol×K	567.84	Joback Method
cpg	199.35	J/mol×K	595.09	Joback Method
cpg	203.67	J/mol×K	622.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50667691&Units=SI

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