1-Methylcyclopropanemethanol

Inchi: InChI=1S/C5H10O/c1-5(4-6)2-3-5/h6H,2-4H2,1H3
InchiKey: PIZQWRXTMGASCZ-UHFFFAOYSA-N
Formula: C5H10O
SMILES: CC1(CO)CC1
Mol. weight [g/mol]: 86.13
CAS: 2746-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-90.34	kJ/mol	Joback Method
hf	-210.72	kJ/mol	Joback Method
hfus	4.63	kJ/mol	Joback Method
hvap	42.16	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.779		Crippen Method
mcvol	76.320	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	394.00 ± 2.00	K	NIST Webbook
tc	595.50	K	Joback Method
tf	258.00 ± 2.00	K	NIST Webbook
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.21	J/mol×K	412.96	Joback Method
cpg	164.04	J/mol×K	443.38	Joback Method
cpg	173.08	J/mol×K	473.81	Joback Method
cpg	181.40	J/mol×K	504.23	Joback Method
cpg	189.10	J/mol×K	534.65	Joback Method
cpg	196.23	J/mol×K	565.08	Joback Method
cpg	202.89	J/mol×K	595.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	401.20	K	100.00	NIST Webbook

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=C2746147&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume