1-Methylcyclohexane-cis-1,2-diol

Inchi: InChI=1S/C7H14O2/c1-7(9)5-3-2-4-6(7)8/h6,8-9H,2-5H2,1H3/t6-,7+/m0/s1
InchiKey: IOZFUGDROBQPNP-NKWVEPMBSA-N
Formula: C7H14O2
SMILES: CC1(O)CCCCC1O
Mol. weight [g/mol]: 130.18
CAS: 52718-65-7

Physical Properties

Property code	Value	Unit	Source
chs	-4147.00 ± 0.80	kJ/mol	NIST Webbook
gf	-254.33	kJ/mol	Joback Method
hf	-443.05	kJ/mol	Joback Method
hfus	8.67	kJ/mol	Joback Method
hvap	63.50	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.672		Crippen Method
mcvol	110.370	ml/mol	McGowan Method
pc	4510.35	kPa	Joback Method
tb	559.04	K	Joback Method
tc	748.16	K	Joback Method
tf	317.33	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.80	J/mol×K	559.04	Joback Method
cpg	297.47	J/mol×K	590.56	Joback Method
cpg	308.51	J/mol×K	622.08	Joback Method
cpg	318.98	J/mol×K	653.60	Joback Method
cpg	328.96	J/mol×K	685.12	Joback Method
cpg	338.52	J/mol×K	716.64	Joback Method
cpg	347.72	J/mol×K	748.16	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=C52718657&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
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