1-Methylcyclooctanol

Other names: Cyclooctanol, 1-methyl-
Inchi: InChI=1S/C9H18O/c1-9(10)7-5-3-2-4-6-8-9/h10H,2-8H2,1H3
InchiKey: YCICXFIRAMLYDV-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CC1(O)CCCCCCC1
Mol. weight [g/mol]: 142.24
CAS: 59123-41-0

Physical Properties

Property code	Value	Unit	Source
gf	-117.16	kJ/mol	Joback Method
hf	-324.08	kJ/mol	Joback Method
hfus	4.49	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.482		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	1121.00		NIST Webbook
rinpol	1121.00		NIST Webbook
tb	525.83	K	Joback Method
tc	736.10	K	Joback Method
tf	308.00 ± 3.00	K	NIST Webbook
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.43	J/mol×K	525.83	Joback Method
cpg	338.80	J/mol×K	560.88	Joback Method
cpg	355.13	J/mol×K	595.92	Joback Method
cpg	370.52	J/mol×K	630.97	Joback Method
cpg	385.05	J/mol×K	666.01	Joback Method
cpg	398.82	J/mol×K	701.06	Joback Method

cpg	411.92	J/mol×K	736.10	Joback Method

Sources

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=C59123410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume