1-Methylcycloheptanol

Other names:	1-Methylcycloheptanol-1
	Cycloheptanol, 1-methyl-
	Methylcycloheptanol-1
	1-methylcycloheptan-1-ol
Inchi:	InChI=1S/C8H16O/c1-8(9)6-4-2-3-5-7-8/h9H,2-7H2,1H3
InchiKey:	XFFKAYOHINCUNU-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CC1(O)CCCCCC1
Mol. weight [g/mol]:	128.21
CAS:	3761-94-2

Physical Properties

Property code	Value	Unit	Source
gf	-113.48	kJ/mol	Joback Method
hf	-297.28	kJ/mol	Joback Method
hfus	4.00	kJ/mol	Joback Method
hvap	49.53	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.092		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
rinpol	1009.00		NIST Webbook
tb	456.70	K	NIST Webbook
tc	704.51	K	Joback Method
tf	268.50	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.86	J/mol×K	498.68	Joback Method
cpg	290.57	J/mol×K	532.98	Joback Method
cpg	305.31	J/mol×K	567.29	Joback Method
cpg	319.15	J/mol×K	601.59	Joback Method

cpg	332.20	J/mol×K	635.90	Joback Method
cpg	344.54	J/mol×K	670.20	Joback Method
cpg	356.27	J/mol×K	704.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3761942&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

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