

1-Methyl-1-cyclohexanecarboxylic acid

Other names:	1-Methyl-1-cyclohexanecarboxylic acid 1-Methylcyclohexanecarboxylic acid Cyclohexanecarboxylic acid, 1-methyl- 1-methylcyclohexane-1-carboxylic acid
Inchi:	InChI=1S/C8H14O2/c1-8(7(9)10)5-3-2-4-6-8/h2-6H2,1H3,(H,9,10)
InchiKey:	REHQLKUNRPCYEW-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CC1(C(=O)O)CCCCC1
Mol. weight [g/mol]:	142.20

Physical Properties

Property code	Value	Unit	Source
af	0.5572		Cheméo Relay (1.0)
gf	-230.30	kJ/mol	Joback Method
hf	-514.51	kJ/mol	Cheméo Relay (1.0)
hfus	7.70	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Cheméo Relay (1.0)
ie	10.09	eV	Cheméo Relay (1.0)
logp	2.041		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
tb	507.20	K	NIST Webbook
tc	717.24	K	Cheméo Relay (1.0)
tf	342.84	K	Cheméo Relay (1.0)
vc	0.408	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.76	J/mol×K	548.28	Joback Method
cpg	308.17	J/mol×K	582.85	Joback Method
cpg	320.73	J/mol×K	617.41	Joback Method
cpg	332.56	J/mol×K	651.98	Joback Method
cpg	343.74	J/mol×K	686.55	Joback Method

cpg	354.38	J/mol×K	721.12	Joback Method
cpg	364.57	J/mol×K	755.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1123257&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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