3-Cyclohexene-1-carboxaldehyde, 4-methyl-

Other names: 1-Cyclohexene-4-carboxaldehyde, 1-methyl-
4-methylcyclohex-3-enecarbaldehyde
3-Cyclohexen-1-carbaldehyde, 4-methyl
Inchi: InChI=1S/C8H12O/c1-7-2-4-8(6-9)5-3-7/h2,6,8H,3-5H2,1H3
InchiKey: YPHGCKOZJCGDTF-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CC1=CCC(C=O)CC1
Mol. weight [g/mol]: 124.18
CAS: 7560-64-7

Physical Properties

Property code	Value	Unit	Source
gf	-38.26	kJ/mol	Joback Method
hf	-193.40	kJ/mol	Joback Method
hfus	11.43	kJ/mol	Joback Method
hvap	41.51	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.932		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	1024.00		NIST Webbook
rinpol	1024.00		NIST Webbook
tb	454.79	K	Joback Method
tc	665.87	K	Joback Method
tf	242.58	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.03	J/mol×K	454.79	Joback Method
cpg	239.42	J/mol×K	489.97	Joback Method
cpg	253.07	J/mol×K	525.15	Joback Method
cpg	265.99	J/mol×K	560.33	Joback Method

cpg	278.20	J/mol×K	595.51	Joback Method
cpg	289.71	J/mol×K	630.69	Joback Method
cpg	300.56	J/mol×K	665.87	Joback Method
dvisc	0.0034828	Pa×s	242.58	Joback Method
dvisc	0.0018235	Pa×s	277.95	Joback Method
dvisc	0.0011049	Pa×s	313.32	Joback Method
dvisc	0.0007411	Pa×s	348.68	Joback Method
dvisc	0.0005350	Pa×s	384.05	Joback Method
dvisc	0.0004081	Pa×s	419.42	Joback Method
dvisc	0.0003246	Pa×s	454.79	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7560647&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
dvisc: Dynamic viscosity
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

Latest version available from: