ISOCYCLOCITRAL

Other names: 3-Cyclohexene-1-carboxaldehyde, 2,4,6-trimethyl-, and 3,5,6-trimethyl-3-cyclohexene-1-carboxaldehyde
1-Formyl-3,5,6-trimethyl-3-cyclohexene and 1-formyl-2,4,6-trimethyl-3-cyclohexene

Inchi: InChI=1S/C10H16O/c1-7-4-8(2)9(3)10(5-7)6-11/h4,6,8-10H,5H2,1-3H3

InchiKey: DEMWVPUIZCCHPT-UHFFFAOYSA-N

Formula: C10H16O

SMILES: CC1=CC(C)C(C)C(C=O)C1

Mol. weight [g/mol]: 152.24

Physical Properties

Property code	Value	Unit	Source
hfus	18.75	kJ/mol	Joback Method
logp	2.424		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
rinpol	1119.90		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1117.00		NIST Webbook
ripol	1515.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.91	J/mol×K	491.21	Joback Method
cpg	331.02	J/mol×K	525.34	Joback Method
cpg	347.33	J/mol×K	559.47	Joback Method
cpg	362.84	J/mol×K	593.59	Joback Method
cpg	377.58	J/mol×K	627.72	Joback Method
cpg	391.54	J/mol×K	661.85	Joback Method
cpg	404.74	J/mol×K	695.98	Joback Method
dvisc	0.0018898	Pa×s	256.64	Joback Method
dvisc	0.0011726	Pa×s	295.74	Joback Method
dvisc	0.0008133	Pa×s	334.83	Joback Method
dvisc	0.0006090	Pa×s	373.92	Joback Method
dvisc	0.0004817	Pa×s	413.02	Joback Method
dvisc	0.0003967	Pa×s	452.12	Joback Method

dvisc	0.0003370	Pa×s	491.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1335666&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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