

3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl-

Other names:	1,3,4-Trimethyl-3-cyclohexenyl-1-carboxaldehyde 1,3,4-Trimethyl-3-cyclohexen-1-carboxaldehyde 1,3,4-Trimethyl-3-cyclohexene-1-carboxaldehyde
Inchi:	InChI=1S/C10H16O/c1-8-4-5-10(3,7-11)6-9(8)2/h7H,4-6H2,1-3H3
InchiKey:	HPPUQZZCHCEJEW-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1=C(C)CC(C)(C=O)CC1
Mol. weight [g/mol]:	152.23
CAS:	40702-26-9

Physical Properties

Property code	Value	Unit	Source
gf	-36.54	kJ/mol	Joback Method
hf	-230.91	kJ/mol	Joback Method
hfus	9.93	kJ/mol	Joback Method
hvap	45.47	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.712		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1136.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1171.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1525.00		NIST Webbook
tb	505.77	K	Joback Method
tc	720.94	K	Joback Method
tf	301.54	K	Joback Method
vc	0.529	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.28	J/mol×K	505.77	Joback Method

cpg	329.19	J/mol×K	541.63	Joback Method
cpg	344.11	J/mol×K	577.49	Joback Method
cpg	358.15	J/mol×K	613.35	Joback Method
cpg	371.41	J/mol×K	649.21	Joback Method
cpg	383.99	J/mol×K	685.08	Joback Method
cpg	396.00	J/mol×K	720.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40702269&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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