

3-Cyclohexenyl-1-acetaldehyde, «alpha»,3-dimethyl

Inchi:	InChI=1S/C10H16O/c1-8-4-3-5-10(6-8)9(2)7-11/h4,7,9-10H,3,5-6H2,1-2H3
InchiKey:	IAKGLPCRKSMZOB-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1=CCCC(C(C)C=O)C1
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	-23.86	kJ/mol	Joback Method
hf	-239.96	kJ/mol	Joback Method
hfus	13.09	kJ/mol	Joback Method
hvap	45.57	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1152.00		NIST Webbook
rinpol	1152.00		NIST Webbook
tb	500.11	K	Joback Method
tc	710.00	K	Joback Method
tf	250.12	K	Joback Method
vc	0.525	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.82	J/mol×K	500.11	Joback Method
cpg	329.63	J/mol×K	535.09	Joback Method
cpg	345.55	J/mol×K	570.07	Joback Method
cpg	360.59	J/mol×K	605.06	Joback Method
cpg	374.78	J/mol×K	640.04	Joback Method
cpg	388.15	J/mol×K	675.02	Joback Method
cpg	400.72	J/mol×K	710.00	Joback Method
dvisc	0.0053140	Paxs	250.12	Joback Method

dvisc	0.0023094	Paxs	291.78	Joback Method
dvisc	0.0012360	Paxs	333.45	Joback Method
dvisc	0.0007601	Paxs	375.12	Joback Method
dvisc	0.0005151	Paxs	416.78	Joback Method
dvisc	0.0003747	Paxs	458.44	Joback Method
dvisc	0.0002874	Paxs	500.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R127869&Units=SI

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

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