

Cyclohexanepropanal

Other names:	Cyclohexanepropionaldehyde 3-Cyclohexylpropionaldehyde
Inchi:	InChI=1S/C9H16O/c10-8-4-7-9-5-2-1-3-6-9/h8-9H,1-7H2
InchiKey:	RKFNAZGRJVNWEW-UHFFFAOYSA-N
Formula:	C9H16O
SMILES:	O=CCCC1CCCCC1
Mol. weight [g/mol]:	140.22
CAS:	4361-28-8

Physical Properties

Property code	Value	Unit	Source
gf	-50.17	kJ/mol	Joback Method
hf	-260.35	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	42.78	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.546		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
tb	473.53	K	Joback Method
tc	678.35	K	Joback Method
tf	240.57	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.85	J/mol×K	473.53	Joback Method
cpg	299.94	J/mol×K	507.67	Joback Method
cpg	316.13	J/mol×K	541.80	Joback Method
cpg	331.45	J/mol×K	575.94	Joback Method
cpg	345.94	J/mol×K	610.08	Joback Method
cpg	359.61	J/mol×K	644.22	Joback Method
cpg	372.48	J/mol×K	678.35	Joback Method

dvisc	0.0068852	Pa×s	240.57	Joback Method
dvisc	0.0029372	Pa×s	279.40	Joback Method
dvisc	0.0015425	Pa×s	318.22	Joback Method
dvisc	0.0009319	Pa×s	357.05	Joback Method
dvisc	0.0006215	Pa×s	395.88	Joback Method
dvisc	0.0004456	Pa×s	434.70	Joback Method
dvisc	0.0003374	Pa×s	473.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.20	K	2.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4361288&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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