

3-Cyclohexene-1-acetaldehyde

Inchi:	InChI=1S/C8H12O/c9-7-6-8-4-2-1-3-5-8/h1-2,7-8H,3-6H2
InchiKey:	UPVGDGITFOERJA-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	O=CCC1CC=CCC1
Mol. weight [g/mol]:	124.18
CAS:	24480-99-7

Physical Properties

Property code	Value	Unit	Source
gf	-28.63	kJ/mol	Joback Method
hf	-181.93	kJ/mol	Joback Method
hfus	11.82	kJ/mol	Joback Method
hvap	40.84	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.932		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	449.81	K	Joback Method
tc	659.50	K	Joback Method
tf	230.06	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.09	J/molxK	449.81	Joback Method
cpg	238.96	J/molxK	484.76	Joback Method
cpg	253.01	J/molxK	519.71	Joback Method
cpg	266.27	J/molxK	554.66	Joback Method
cpg	278.77	J/molxK	589.61	Joback Method
cpg	290.52	J/molxK	624.55	Joback Method
cpg	301.56	J/molxK	659.50	Joback Method
dvisc	0.0052247	Paxs	230.06	Joback Method
dvisc	0.0024264	Paxs	266.69	Joback Method

dvisc	0.0013561	Paxs	303.31	Joback Method
dvisc	0.0008592	Paxs	339.93	Joback Method
dvisc	0.0005949	Paxs	376.56	Joback Method
dvisc	0.0004396	Paxs	413.18	Joback Method
dvisc	0.0003413	Paxs	449.81	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24480997&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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