

1-Cyclohexenylacetic acid

Other names:	1-Cyclohexene-1-acetic acid cyclohex-1-enylacetic acid
Inchi:	InChI=1S/C8H12O2/c9-8(10)6-7-4-2-1-3-5-7/h4H,1-3,5-6H2,(H,9,10)
InchiKey:	KDFBPHXESBPHTK-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	O=C(O)CC1=CCCCC1
Mol. weight [g/mol]:	140.18
CAS:	18294-87-6

Physical Properties

Property code	Value	Unit	Source
gf	-196.77	kJ/mol	Joback Method
hf	-352.29	kJ/mol	Joback Method
hfus	13.76	kJ/mol	Joback Method
hvap	58.52	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.962		Crippen Method
mvol	115.860	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	556.85	K	Joback Method
tc	759.39	K	Joback Method
tf	315.57	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.73	J/molxK	556.85	Joback Method
cpg	327.73	J/molxK	725.63	Joback Method
cpg	318.40	J/molxK	691.88	Joback Method
cpg	308.45	J/molxK	658.12	Joback Method
cpg	297.88	J/molxK	624.36	Joback Method
cpg	286.64	J/molxK	590.61	Joback Method
cpg	336.47	J/molxK	759.39	Joback Method

dvisc	0.0001231	Paxs	556.85	Joback Method
dvisc	0.0001940	Paxs	516.64	Joback Method
dvisc	0.0003301	Paxs	476.42	Joback Method
dvisc	0.0006197	Paxs	436.21	Joback Method
dvisc	0.0013219	Paxs	396.00	Joback Method
dvisc	0.0033466	Paxs	355.78	Joback Method
dvisc	0.0107359	Paxs	315.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.00 ± 1.00	K	3.30	NIST Webbook

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=C18294876&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
mccvol:	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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