Cyclohexyl propionate

Other names:	Cyclohexyl n-propionate
	Propionic acid cyclohexyl ester
	cyclohexyl propanoate
	propanoic acid, cyclohexyl ester
	propionic acid, cyclohexyl ester
Inchi:	InChI=1S/C9H16O2/c1-2-9(10)11-8-6-4-3-5-7-8/h8H,2-7H2,1H3
InchiKey:	MAMMVUWCKMOLSG-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	CCC(=O)OC1CCCCC1
Mol. weight [g/mol]:	156.22
CAS:	6222-35-1

Physical Properties

Property code	Value	Unit	Source
gf	-184.57	kJ/mol	Joback Method
hf	-419.57	kJ/mol	Joback Method
hfus	13.69	kJ/mol	Joback Method
hvap	56.80	kJ/mol	NIST Webbook
hvap	55.90 ± 0.10	kJ/mol	NIST Webbook
hvap	59.40 ± 0.80	kJ/mol	NIST Webbook
hvap	56.40 ± 0.50	kJ/mol	NIST Webbook
hvap	54.30 ± 0.40	kJ/mol	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.272		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1120.00		NIST Webbook
rinpol	1111.00		NIST Webbook
ripol	1408.00		NIST Webbook
tb	501.16	K	Joback Method
tc	709.61	K	Joback Method
tf	270.73	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.17	J/mol×K	709.61	Joback Method
cpg	308.34	J/mol×K	501.16	Joback Method
cpg	325.39	J/mol×K	535.90	Joback Method
cpg	341.59	J/mol×K	570.64	Joback Method
cpg	356.96	J/mol×K	605.38	Joback Method
cpg	371.51	J/mol×K	640.12	Joback Method
cpg	385.24	J/mol×K	674.87	Joback Method
dvisc	0.0002611	Pa×s	501.16	Joback Method
dvisc	0.0043071	Pa×s	270.73	Joback Method
dvisc	0.0020196	Pa×s	309.13	Joback Method
dvisc	0.0011196	Pa×s	347.54	Joback Method
dvisc	0.0006979	Pa×s	385.94	Joback Method
dvisc	0.0004740	Pa×s	424.35	Joback Method
dvisc	0.0003432	Pa×s	462.75	Joback Method
hvapt	55.73	kJ/mol	300.55	Comprehensive Study of Vapor Pressures and Enthalpies of Vaporization of Cyclohexyl Esters

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Comprehensive Study of Vapor Pressures and Enthalpies of Vaporization of Cyclohexyl Esters: https://www.doi.org/10.1021/je025634v

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=C6222351&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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume