

2-propenoic acid, cyclohexyl ester

Other names:	cyclohexyl 2-propenoate
Inchi:	InChI=1S/C9H14O2/c1-2-9(10)11-8-6-4-3-5-7-8/h2,8H,1,3-7H2
InchiKey:	KBLWLMPSVYBVDK-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	C=CC(=O)OC1CCCCC1
Mol. weight [g/mol]:	154.21

Physical Properties

Property code	Value	Unit	Source
hf	-390.15	kJ/mol	Cheméo Relay (1.0)
hfus	12.41	kJ/mol	Joback Method
hvap	55.83	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.48		Cheméo Relay (1.0)
logp	2.048		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
tb	461.53	K	Cheméo Relay (1.0)
tf	229.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.18	J/mol×K	497.84	Joback Method
cpg	306.62	J/mol×K	533.35	Joback Method
cpg	322.19	J/mol×K	568.85	Joback Method
cpg	336.91	J/mol×K	604.36	Joback Method
cpg	350.78	J/mol×K	639.86	Joback Method
cpg	363.84	J/mol×K	675.37	Joback Method
cpg	376.08	J/mol×K	710.87	Joback Method
dvisc	0.0039825	Pa×s	268.97	Joback Method
dvisc	0.0019153	Pa×s	307.12	Joback Method
dvisc	0.0010828	Pa×s	345.26	Joback Method
dvisc	0.0006858	Pa×s	383.41	Joback Method
dvisc	0.0004717	Pa×s	421.55	Joback Method
dvisc	0.0003453	Pa×s	459.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Phase Behavior of the Binary Mixture of Cyclohexyl Acrylate and Cyclohexyl Methacrylate in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je0497707
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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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