

Cyclohexanecarboxylic acid, ethenyl ester

Other names:	Cyclohexanecarboxylic acid, vinyl ester Vinyl cyclohexanecarboxylate
Inchi:	InChI=1S/C9H14O2/c1-2-11-9(10)8-6-4-3-5-7-8/h2,8H,1,3-7H2
InchiKey:	JZRGFKQYQJGAK-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	C=COC(=O)C1CCCCC1
Mol. weight [g/mol]:	154.21
CAS:	4840-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-96.73	kJ/mol	Joback Method
hf	-294.14	kJ/mol	Joback Method
hfus	12.41	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.253		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	1137.00		NIST Webbook
rinpol	1137.00		NIST Webbook
tb	497.84	K	Joback Method
tc	710.87	K	Joback Method
tf	268.97	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.18	J/molxK	497.84	Joback Method
cpg	363.84	J/molxK	675.37	Joback Method
cpg	350.78	J/molxK	639.86	Joback Method
cpg	336.91	J/molxK	604.36	Joback Method
cpg	322.19	J/molxK	568.85	Joback Method

cpg	306.62	J/mol×K	533.35	Joback Method
cpg	376.08	J/mol×K	710.87	Joback Method
dvisc	0.0002651	Paxs	497.84	Joback Method
dvisc	0.0003453	Paxs	459.70	Joback Method
dvisc	0.0004717	Paxs	421.55	Joback Method
dvisc	0.0006858	Paxs	383.41	Joback Method
dvisc	0.0010828	Paxs	345.26	Joback Method
dvisc	0.0019153	Paxs	307.12	Joback Method
dvisc	0.0039825	Paxs	268.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4840760&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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