Formic acid, cyclohexyl ester

Other names:	Cyclohexyl ester of formic acid
	Formic acid, cyclohexyl ester (purified)
	cyclohexyl formate
	cyclohexyl methanoate
	methanoic acid, cyclohexyl ester
Inchi:	InChI=1S/C7H12O2/c8-6-9-7-4-2-1-3-5-7/h6-7H,1-5H2
InchiKey:	VUXKVKAHWOVIDN-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	O=COC1CCCCC1
Mol. weight [g/mol]:	128.17
CAS:	4351-54-6

Physical Properties

Property code	Value	Unit	Source
gf	-172.01	kJ/mol	Joback Method
hf	-351.29	kJ/mol	Joback Method
hfus	9.20	kJ/mol	Joback Method
hvap	49.30 ± 0.20	kJ/mol	NIST Webbook
hvap	52.00 ± 1.30	kJ/mol	NIST Webbook
hvap	49.50 ± 1.20	kJ/mol	NIST Webbook
log10ws	-1.62		Crippen Method
logp	1.492		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	951.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1304.00		NIST Webbook
tb	450.19	K	Joback Method
tc	659.00	K	Joback Method
tf	240.26	K	Joback Method
tt	201.33 ± 0.15	K	NIST Webbook
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.48	J/mol×K	624.20	Joback Method
cpg	298.70	J/mol×K	659.00	Joback Method
cpg	221.35	J/mol×K	450.19	Joback Method
cpg	235.94	J/mol×K	484.99	Joback Method
cpg	249.84	J/mol×K	519.79	Joback Method
cpg	263.06	J/mol×K	554.59	Joback Method
cpg	275.61	J/mol×K	589.40	Joback Method
dvisc	0.0004121	Pa×s	415.20	Joback Method
dvisc	0.0003166	Pa×s	450.19	Joback Method
dvisc	0.0048731	Pa×s	240.26	Joback Method
dvisc	0.0023129	Pa×s	275.25	Joback Method
dvisc	0.0012987	Pa×s	310.24	Joback Method
dvisc	0.0008197	Pa×s	345.23	Joback Method
dvisc	0.0005631	Pa×s	380.21	Joback Method
hfust	10.49	kJ/mol	201.30	NIST Webbook
hvapt	47.10	kJ/mol	370.50	NIST Webbook
hvapt	48.82	kJ/mol	303.52	Comprehensive Study of Vapor Pressures and Enthalpies of Vaporization of Cyclohexyl Esters

Sources

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=C4351546&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurements and Correlation of Liquid-Liquid Equilibria for the Ternary System Cyclohexanol + Water + Cyclohexyl Formate at 298.2-338.2 K:	https://www.doi.org/10.1021/acs.jced.8b01104
Comprehensive Study of Vapor Pressures and Enthalpies of Vaporization of Cyclohexyl Esters:	https://www.doi.org/10.1021/je025634v

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
hfust:	Enthalpy of fusion at a given temperature
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
tt:	Triple Point Temperature
vc:	Critical Volume