

Formic acid, cycloheptyl ester

Inchi:	InChI=1S/C8H14O2/c9-7-10-8-5-3-1-2-4-6-8/h7-8H,1-6H2
InchiKey:	KQPTVERBLKLHLD-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	O=COC1CCCCC1
Mol. weight [g/mol]:	142.20
CAS:	75024-32-7

Physical Properties

Property code	Value	Unit	Source
gf	-175.69	kJ/mol	Joback Method
hf	-378.09	kJ/mol	Joback Method
hfus	9.69	kJ/mol	Joback Method
hvap	43.13	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.882		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
tb	477.34	K	Joback Method
tc	691.44	K	Joback Method
tf	248.01	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.75	J/molxK	477.34	Joback Method
cpg	280.44	J/molxK	513.02	Joback Method
cpg	296.32	J/molxK	548.71	Joback Method
cpg	311.40	J/molxK	584.39	Joback Method
cpg	325.67	J/molxK	620.07	Joback Method
cpg	339.14	J/molxK	655.76	Joback Method
cpg	351.80	J/molxK	691.44	Joback Method
dvisc	0.0070032	Paxs	248.01	Joback Method
dvisc	0.0027799	Paxs	286.23	Joback Method

dvisc	0.0013718	Paxs	324.45	Joback Method
dvisc	0.0007856	Paxs	362.67	Joback Method
dvisc	0.0005004	Paxs	400.90	Joback Method
dvisc	0.0003447	Paxs	439.12	Joback Method
dvisc	0.0002521	Paxs	477.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75024327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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