

Formic acid, trans-4-methylcyclohexyl ester

Inchi:	InChI=1S/C8H14O2/c1-7-2-4-8(5-3-7)10-6-9/h6-8H,2-5H2,1H3
InchiKey:	DZRDTGDYROJVPD-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CC1CCC(OC=O)CC1
Mol. weight [g/mol]:	142.20

Physical Properties

Property code	Value	Unit	Source
gf	-171.30	kJ/mol	Joback Method
hf	-392.27	kJ/mol	Joback Method
hfus	12.86	kJ/mol	Joback Method
hvap	42.65	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.738		Crippen Method
mvol	120.160	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	1026.00		NIST Webbook
rinpol	1026.00		NIST Webbook
tb	468.40	K	Joback Method
tc	674.15	K	Joback Method
tf	247.29	K	Joback Method
vc	0.451	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.74	J/mol×K	468.40	Joback Method
cpg	280.75	J/mol×K	502.69	Joback Method
cpg	296.05	J/mol×K	536.98	Joback Method
cpg	310.62	J/mol×K	571.28	Joback Method
cpg	324.48	J/mol×K	605.57	Joback Method
cpg	337.63	J/mol×K	639.86	Joback Method
cpg	350.06	J/mol×K	674.15	Joback Method
dvisc	0.0034215	Paxs	247.29	Joback Method

dvisc	0.0017716	Paxs	284.14	Joback Method
dvisc	0.0010669	Paxs	320.99	Joback Method
dvisc	0.0007133	Paxs	357.85	Joback Method
dvisc	0.0005141	Paxs	394.70	Joback Method
dvisc	0.0003919	Paxs	431.55	Joback Method
dvisc	0.0003117	Paxs	468.40	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368245&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
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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