

trans-Vetrocital C

Inchi:	InChI=1S/C9H14O/c1-7-3-4-9(6-10)8(2)5-7/h5-6,8-9H,3-4H2,1-2H3/t8-,9+/m0/s1
InchiKey:	MZZRKEIUNOYYDF-DTWKUNHWSA-N
Formula:	C9H14O
SMILES:	CC1=CC(C)C(C=O)CC1
Mol. weight [g/mol]:	138.21

Physical Properties

Property code	Value	Unit	Source
gf	-37.55	kJ/mol	Joback Method
hf	-234.38	kJ/mol	Joback Method
hfus	15.09	kJ/mol	Joback Method
hvap	43.42	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.178		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	1101.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1102.00		NIST Webbook
tb	473.00	K	Joback Method
tc	680.91	K	Joback Method
tf	249.61	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.51	J/mol×K	473.00	Joback Method
cpg	339.93	J/mol×K	646.26	Joback Method
cpg	327.13	J/mol×K	611.61	Joback Method
cpg	313.61	J/mol×K	576.96	Joback Method
cpg	299.34	J/mol×K	542.30	Joback Method
cpg	284.31	J/mol×K	507.65	Joback Method
cpg	352.00	J/mol×K	680.91	Joback Method

dvisc	0.0003273	Pa×s	473.00	Joback Method
dvisc	0.0003978	Pa×s	435.77	Joback Method
dvisc	0.0005014	Pa×s	398.54	Joback Method
dvisc	0.0006629	Pa×s	361.31	Joback Method
dvisc	0.0009346	Pa×s	324.07	Joback Method
dvisc	0.0014404	Pa×s	286.84	Joback Method
dvisc	0.0025258	Pa×s	249.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R288018&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
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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