

L-carvenyl acetate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)12(7-11)14-10(4)13/h7-9,12H,5-6H2,1-4H3

KLARWHVPTTYEW-UHFFFAOYSA-N

C12H20O2

CC(=O)OC1C=C(C(C)C)CCC1C

196.29

Physical Properties

Property code	Value	Unit	Source
gf	-149.13	kJ/mol	Joback Method
hf	-460.80	kJ/mol	Joback Method
hfus	19.84	kJ/mol	Joback Method
hvap	52.15	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.930		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
ripol	1734.00		NIST Webbook
ripol	1731.00		NIST Webbook
tb	568.83	K	Joback Method
tc	775.12	K	Joback Method
tf	298.58	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.48	J/mol×K	568.83	Joback Method
cpg	455.12	J/mol×K	603.21	Joback Method
cpg	472.81	J/mol×K	637.59	Joback Method
cpg	489.57	J/mol×K	671.97	Joback Method
cpg	505.41	J/mol×K	706.36	Joback Method
cpg	520.32	J/mol×K	740.74	Joback Method
cpg	534.32	J/mol×K	775.12	Joback Method
dvisc	0.0025980	Pa×s	298.58	Joback Method

dvisc	0.0013006	Pa×s	343.62	Joback Method
dvisc	0.0007644	Pa×s	388.66	Joback Method
dvisc	0.0005017	Pa×s	433.71	Joback Method
dvisc	0.0003564	Pa×s	478.75	Joback Method
dvisc	0.0002685	Pa×s	523.79	Joback Method
dvisc	0.0002116	Pa×s	568.83	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R330931&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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