

Sesquichamaenol (1,10-seco-1-hydroxycalamenen-10-one)

Inchi:	InChI=1S/C14H20O2/c1-10(2)12(9-8-11(3)15)13-6-4-5-7-14(13)16/h4-7,10,12,16H,8-9H2
InchiKey:	PMIDBMKKOYSBHF-LBPRGKRZSA-N
Formula:	C14H20O2
SMILES:	CC(=O)CCC(c1cccc1O)C(C)C
Mol. weight [g/mol]:	220.31

Physical Properties

Property code	Value	Unit	Source
gf	-109.01	kJ/mol	Joback Method
hf	-396.21	kJ/mol	Joback Method
hfus	26.39	kJ/mol	Joback Method
hvap	68.02	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.501		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1748.00		NIST Webbook
ripol	2681.00		NIST Webbook
tb	680.01	K	Joback Method
tc	899.26	K	Joback Method
tf	405.61	K	Joback Method
vc	0.671	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.96	J/mol×K	680.01	Joback Method
cpg	541.42	J/mol×K	716.55	Joback Method
cpg	555.93	J/mol×K	753.09	Joback Method
cpg	569.57	J/mol×K	789.63	Joback Method
cpg	582.42	J/mol×K	826.17	Joback Method
cpg	594.58	J/mol×K	862.71	Joback Method
cpg	606.13	J/mol×K	899.26	Joback Method
dvisc	0.0014306	Paxs	405.61	Joback Method

dvisc	0.0004652	Paxs	451.34	Joback Method
dvisc	0.0001860	Paxs	497.08	Joback Method
dvisc	0.0000868	Paxs	542.81	Joback Method
dvisc	0.0000456	Paxs	588.54	Joback Method
dvisc	0.0000263	Paxs	634.28	Joback Method
dvisc	0.0000163	Paxs	680.01	Joback Method

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=R229024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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
vc:	Critical Volume

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