Sesquichamaenol

Inchi: InChI=1S/C15H22O2/c1-10(2)13(7-6-12(4)16)14-9-11(3)5-8-15(14)17/h5,8-10,13,17H,6-
InchiKey: UFWXDPOVAJYDEP-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CC(=O)CCC(c1cc(C)ccc1O)C(C)C
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-110.22	kJ/mol	Joback Method
hf	-428.32	kJ/mol	Joback Method
hfus	28.59	kJ/mol	Joback Method
hvap	70.91	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.809		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1745.00		NIST Webbook
rinpol	1745.00		NIST Webbook
ripol	2683.00		NIST Webbook
ripol	2683.00		NIST Webbook
tb	707.87	K	Joback Method
tc	924.44	K	Joback Method
tf	429.40	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.10	J/mol×K	707.87	Joback Method
cpg	593.85	J/mol×K	743.96	Joback Method
cpg	608.69	J/mol×K	780.06	Joback Method
cpg	622.70	J/mol×K	816.15	Joback Method
cpg	635.96	J/mol×K	852.25	Joback Method
cpg	648.55	J/mol×K	888.34	Joback Method

cpg	660.55	J/mol×K	924.44	Joback Method
dvisc	0.0008191	Pa×s	429.40	Joback Method
dvisc	0.0002921	Pa×s	475.81	Joback Method
dvisc	0.0001251	Pa×s	522.22	Joback Method
dvisc	0.0000615	Pa×s	568.63	Joback Method
dvisc	0.0000337	Pa×s	615.05	Joback Method
dvisc	0.0000201	Pa×s	661.46	Joback Method
dvisc	0.0000128	Pa×s	707.87	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=R229722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume