Calamenol 1

Inchi: InChI=1S/C15H22O/c1-9(2)12-7-5-10(3)13-8-6-11(4)15(16)14(12)13/h6,8-10,12,16H,5,7
InchiKey: YXYMGKMWKSMRAB-UHFFFAOYSA-N
Formula: C15H22O
SMILES: Cc1ccc2c(c1O)C(C(C)C)CCC2C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	52.45	kJ/mol	Joback Method
hf	-275.63	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.338		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1657.00		NIST Webbook
tb	665.76	K	Joback Method
tc	893.47	K	Joback Method
tf	417.17	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.17	J/mol×K	665.76	Joback Method
cpg	629.78	J/mol×K	855.52	Joback Method
cpg	615.14	J/mol×K	817.56	Joback Method
cpg	599.66	J/mol×K	779.61	Joback Method
cpg	583.24	J/mol×K	741.66	Joback Method
cpg	565.78	J/mol×K	703.71	Joback Method
cpg	643.69	J/mol×K	893.47	Joback Method
dvisc	0.0000379	Pa×s	665.76	Joback Method
dvisc	0.0000546	Pa×s	624.33	Joback Method

dvisc	0.0000827	Pa×s	582.90	Joback Method
dvisc	0.0001337	Pa×s	541.47	Joback Method
dvisc	0.0002338	Pa×s	500.03	Joback Method
dvisc	0.0004524	Pa×s	458.60	Joback Method
dvisc	0.0009983	Pa×s	417.17	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=R517683&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume