Pacifigorgiol

Inchi: InChI=1S/C15H26O/c1-10(2)9-14-11(3)5-6-13-12(4)7-8-15(13,14)16/h9,11-14,16H,5-8H2
InchiKey: QGALFKRHZSPTEG-UHFFFAOYSA-N
Formula: C15H26O
SMILES: CC(C)=CC1C(C)CCC2C(C)CCC12O
Mol. weight [g/mol]: 222.37
CAS: 84014-68-6

Physical Properties

Property code	Value	Unit	Source
gf	66.85	kJ/mol	Joback Method
hf	-316.39	kJ/mol	Joback Method
hfus	24.47	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	1556.80		NIST Webbook
rinpol	1552.00		NIST Webbook
tb	651.34	K	Joback Method
tc	854.93	K	Joback Method
tf	337.09	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.46	J/mol×K	651.34	Joback Method
cpg	617.70	J/mol×K	685.27	Joback Method
cpg	636.91	J/mol×K	719.20	Joback Method
cpg	655.21	J/mol×K	753.14	Joback Method
cpg	672.74	J/mol×K	787.07	Joback Method
cpg	689.62	J/mol×K	821.00	Joback Method
cpg	705.99	J/mol×K	854.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84014686&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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