

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-CMTGQMGJSA-N
Formula:	C15H26O
SMILES:	CC(C)=CC1C(C)CCC2C(C)CCC12O
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
hfus	24.47	kJ/mol	Joback Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1540.40		NIST Webbook
rinpol	1523.00		NIST Webbook

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

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook:
Joback Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R196251&Units=SI>
https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
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
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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