7-epi-«alpha»-Eudesmol

Inchi: InChI=1S/C15H26O/c1-11-6-5-8-15(4)9-7-12(10-13(11)15)14(2,3)16/h6,12-13,16H,5,7-1
InchiKey: FCSRUSQUAVXUKK-NFAWXSAZSA-N
Formula: C15H26O
SMILES: CC1=CCCC2(C)CCC(C(C)(C)O)CC12
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	14.76	kJ/mol	Joback Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1657.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1653.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook

rinpol	1663.00	NIST Webbook
ripol	2244.00	NIST Webbook
ripol	2244.00	NIST Webbook
ripol	2205.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.13	J/mol×K	661.82	Joback Method
cpg	618.08	J/mol×K	697.19	Joback Method
cpg	636.92	J/mol×K	732.57	Joback Method
cpg	654.81	J/mol×K	767.94	Joback Method
cpg	671.91	J/mol×K	803.32	Joback Method
cpg	688.38	J/mol×K	838.69	Joback Method
cpg	704.35	J/mol×K	874.07	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R203933&Units=SI

Joback Method: 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

Cheméo Relay (1.0):

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

ripol: Polar retention indices