(-)-2,3,3a,4,5,6-Hexahydro-1,4-dimethylazulen-4-ol

Inchi: InChI=1S/C12H18O/c1-9-6-7-11-10(9)5-3-4-8-12(11,2)13/h3,5,11,13H,4,6-8H2,1-2H3
InchiKey: RZOQSQQQVAELHL-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC1=C2C=CCCC(C)(O)C2CC1
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	21.61	kJ/mol	Joback Method
hf	-214.42	kJ/mol	Joback Method
hfus	14.16	kJ/mol	Joback Method
hvap	60.26	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.814		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
tb	605.22	K	Joback Method
tc	818.89	K	Joback Method
tf	358.08	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.82	J/mol×K	605.22	Joback Method
cpg	429.98	J/mol×K	640.83	Joback Method
cpg	445.20	J/mol×K	676.44	Joback Method
cpg	459.61	J/mol×K	712.05	Joback Method
cpg	473.33	J/mol×K	747.66	Joback Method
cpg	486.51	J/mol×K	783.28	Joback Method
cpg	499.27	J/mol×K	818.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515716&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

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