

Azulen-2-ol, 1,4-dimethyl-7-(1-methylethyl)-

Other names:	1,4-Dimethyl-7-(1-methylethyl)-azulene-2-ol
Inchi:	InChI=1S/C15H18O/c1-9(2)12-6-5-10(3)13-8-15(16)11(4)14(13)7-12/h5-9,16H,1-4H3
InchiKey:	GYTYRDSGJDMKCK-UHFFFAOYSA-N
Formula:	C15H18O
SMILES:	<chem>Cc1ccc(C(C)C)cc2c(C)c(O)cc1-2</chem>
Mol. weight [g/mol]:	214.30
CAS:	18937-66-1

Physical Properties

Property code	Value	Unit	Source
gf	108.53	kJ/mol	Joback Method
hf	-142.33	kJ/mol	Joback Method
hfus	26.76	kJ/mol	Joback Method
hvap	67.51	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.237		Crippen Method
mcvol	184.860	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	1934.00		NIST Webbook
tb	683.38	K	Joback Method
tc	916.72	K	Joback Method
tf	452.21	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.14	J/molxK	683.38	Joback Method
cpg	509.24	J/molxK	722.27	Joback Method
cpg	523.44	J/molxK	761.16	Joback Method
cpg	536.84	J/molxK	800.05	Joback Method
cpg	549.58	J/molxK	838.94	Joback Method
cpg	561.76	J/molxK	877.83	Joback Method
cpg	573.50	J/molxK	916.72	Joback Method

dvisc	0.0004772	Paxs	452.21	Joback Method
dvisc	0.0002443	Paxs	490.74	Joback Method
dvisc	0.0001379	Paxs	529.27	Joback Method
dvisc	0.0000841	Paxs	567.80	Joback Method
dvisc	0.0000546	Paxs	606.32	Joback Method
dvisc	0.0000374	Paxs	644.85	Joback Method
dvisc	0.0000267	Paxs	683.38	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=C18937661&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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