Azulene, 1,4-dimethyl-7-(1-methylethyl)-

Other names:	Azulene, 7-isopropyl-1,4-dimethyl-
	Azulen-Beris
	Azulol
	Azulon
	Azunol
	Cuteazul
	Eucazulen
	Guaiazulene
	Gurjunazulen
	Kessazulen
	Purazulen
	S-Guaiazulene
	Silazulon
	Uroazulen
	Vetivazulen
	1,4-Dimethyl-7-isopropylazulene
	3,8-Dimethyl-5-(2-propyl)azulene
	7-Isopropyl-1,4-dimethylazulene
	1,4-Dimethyl-7-(1-methylethyl)azulene
	Azulene, 1,4-dimethyl-7-isopropyl-
	Guajazulene
	Guiazulene
	AZ-8
	AZ-8 beris
	Vaumigan
	NSC 4714
	1,4-dimethyl-7-(1-methyl)-azulene (azulon)
Inchi:	InChI=1S/C15H18/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h5-10H,1-4H3
InchiKey:	FWKQNCXZGNBPFD-UHFFFAOYSA-N
Formula:	C15H18
SMILES:	Cc1ccc(C(C)C)cc2c(C)ccc1-2
Mol. weight [g/mol]:	198.30
CAS:	489-84-9

Physical Properties

Property code	Value	Unit	Source

affp	983.10	kJ/mol	NIST Webbook
basg	950.60	kJ/mol	NIST Webbook
chs	-8536.20 ± 3.80	kJ/mol	NIST Webbook
chs	-8463.80 ± 7.50	kJ/mol	NIST Webbook
gf	263.15	kJ/mol	Joback Method
hf	34.98	kJ/mol	Joback Method
hfus	20.98	kJ/mol	Joback Method
hvap	54.50	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.532		Crippen Method
mcvol	178.990	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1734.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1772.00		NIST Webbook
tb	602.76	K	Joback Method
tc	827.42	K	Joback Method
tf	340.49	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.16	J/mol×K	602.76	Joback Method
cpg	514.60	J/mol×K	789.98	Joback Method
cpg	501.39	J/mol×K	752.54	Joback Method
cpg	487.31	J/mol×K	715.09	Joback Method
cpg	472.29	J/mol×K	677.65	Joback Method
cpg	456.26	J/mol×K	640.20	Joback Method
cpg	526.98	J/mol×K	827.42	Joback Method
dvisc	0.0002427	Pa×s	602.76	Joback Method
dvisc	0.0002889	Pa×s	559.05	Joback Method
dvisc	0.0003542	Pa×s	515.34	Joback Method
dvisc	0.0004510	Pa×s	471.62	Joback Method
dvisc	0.0006032	Pa×s	427.91	Joback Method
dvisc	0.0008620	Pa×s	384.20	Joback Method
dvisc	0.0013500	Pa×s	340.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	426.20	K	0.90	NIST Webbook
tbrp	440.70	K	1.60	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C489849&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume