Azulene, 2,6-dimethyl-4-phenyl

Inchi: InChI=1S/C18H16/c1-13-8-9-16-10-14(2)12-18(16)17(11-13)15-6-4-3-5-7-15/h3-12H,1-2
InchiKey: BAOBEDNJHDPRDX-UHFFFAOYSA-N
Formula: C18H16
SMILES: Cc1ccc2cc(C)cc-2c(-c2ccccc2)c1
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	403.26	kJ/mol	Joback Method
hf	214.87	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	63.84	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	5.075		Crippen Method
mcvol	197.500	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	372.30		NIST Webbook
tb	698.52	K	Joback Method
tc	950.72	K	Joback Method
tf	415.72	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.38	J/mol×K	698.52	Joback Method
cpg	586.71	J/mol×K	908.69	Joback Method
cpg	574.23	J/mol×K	866.66	Joback Method
cpg	560.77	J/mol×K	824.62	Joback Method
cpg	546.22	J/mol×K	782.59	Joback Method
cpg	530.47	J/mol×K	740.55	Joback Method
cpg	598.33	J/mol×K	950.72	Joback Method
dvisc	0.0002205	Pa×s	698.52	Joback Method
dvisc	0.0002608	Pa×s	651.39	Joback Method

dvisc	0.0003167	Pa×s	604.25	Joback Method
dvisc	0.0003974	Pa×s	557.12	Joback Method
dvisc	0.0005200	Pa×s	509.99	Joback Method
dvisc	0.0007187	Pa×s	462.85	Joback Method
dvisc	0.0010690	Pa×s	415.72	Joback Method

Sources

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=R39052&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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