Azulene, 1,2,3-triphenyl-

Other names: 1,2,3-Triphenylazulene
Inchi: InChI=1S/C28H20/c1-5-13-21(14-6-1)26-24-19-11-4-12-20-25(24)27(22-15-7-2-8-16-22)
InchiKey: BBAHZGDEGNYDBK-UHFFFAOYSA-N
Formula: C28H20
SMILES: c1ccc(-c2c3ccccc-3c(-c3ccccc3)c2-c2ccccc2)cc1
Mol. weight [g/mol]: 356.46
CAS: 1055-26-1

Physical Properties

Property code	Value	Unit	Source
gf	712.28	kJ/mol	Joback Method
hf	481.53	kJ/mol	Joback Method
hfus	40.29	kJ/mol	Joback Method
hvap	90.65	kJ/mol	Joback Method
ie	6.90	eV	NIST Webbook
log10ws	-11.30		Crippen Method
logp	7.792		Crippen Method
mcvol	290.880	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
tb	980.68	K	Joback Method
tc	1265.15	K	Joback Method
tf	581.26	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.24	J/mol×K	980.68	Joback Method
cpg	899.15	J/mol×K	1028.09	Joback Method
cpg	914.01	J/mol×K	1075.50	Joback Method
cpg	928.11	J/mol×K	1122.91	Joback Method
cpg	941.71	J/mol×K	1170.33	Joback Method
cpg	955.09	J/mol×K	1217.74	Joback Method
cpg	968.52	J/mol×K	1265.15	Joback Method

dvisc	0.0005280	Pa×s	581.26	Joback Method
dvisc	0.0003317	Pa×s	647.83	Joback Method
dvisc	0.0002273	Pa×s	714.40	Joback Method
dvisc	0.0001661	Pa×s	780.97	Joback Method
dvisc	0.0001275	Pa×s	847.54	Joback Method
dvisc	0.0001017	Pa×s	914.11	Joback Method
dvisc	0.0000837	Pa×s	980.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1055261&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
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume