

Inden-1-ol, 1,2,3-triphenyl-

Inchi:	InChI=1S/C27H20O/c28-27(22-16-8-3-9-17-22)24-19-11-10-18-23(24)25(20-12-4-1-5-13
InchiKey:	ADZZBNYBYSNNGJ-UHFFFAOYSA-N
Formula:	C27H20O
SMILES:	OC1(c2ccccc2)C(c2ccccc2)=C(c2ccccc2)c2ccccc21
Mol. weight [g/mol]:	360.45
CAS:	42454-94-4

Physical Properties

Property code	Value	Unit	Source
gf	545.61	kJ/mol	Joback Method
hf	304.69	kJ/mol	Joback Method
hfus	37.83	kJ/mol	Joback Method
hvap	102.52	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	5.895		Crippen Method
mcvol	286.960	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
tb	1037.14	K	Joback Method
tc	1304.88	K	Joback Method
tf	640.71	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.89	J/molxK	1037.14	Joback Method
cpg	942.50	J/molxK	1081.76	Joback Method
cpg	965.27	J/molxK	1126.39	Joback Method
cpg	989.60	J/molxK	1171.01	Joback Method
cpg	1015.88	J/molxK	1215.64	Joback Method
cpg	1044.52	J/molxK	1260.26	Joback Method
cpg	1075.91	J/molxK	1304.88	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=C42454944&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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