Indan, 1,1,6,7-tetramethyl-

Inchi: InChI=1S/C13H18/c1-9-5-6-11-7-8-13(3,4)12(11)10(9)2/h5-6H,7-8H2,1-4H3
InchiKey: AKAQKGLHKLCCCF-UHFFFAOYSA-N
Formula: C13H18
SMILES: Cc1ccc2c(c1C)C(C)(C)CC2
Mol. weight [g/mol]: 174.28
CAS: 16204-58-3

Physical Properties

Property code	Value	Unit	Source
gf	197.36	kJ/mol	Joback Method
hf	-21.49	kJ/mol	Joback Method
hfus	14.14	kJ/mol	Joback Method
hvap	47.56	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.527		Crippen Method
mcvol	159.410	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
tb	545.44	K	Joback Method
tc	769.28	K	Joback Method
tf	342.09	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.74	J/mol×K	545.44	Joback Method
cpg	397.09	J/mol×K	582.75	Joback Method
cpg	413.31	J/mol×K	620.05	Joback Method
cpg	428.55	J/mol×K	657.36	Joback Method
cpg	442.97	J/mol×K	694.67	Joback Method
cpg	456.71	J/mol×K	731.97	Joback Method
cpg	469.93	J/mol×K	769.28	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=C16204583&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume