1H-Indene, 1,1,3-trimethyl-

Inchi: InChI=1S/C12H14/c1-9-8-12(2,3)11-7-5-4-6-10(9)11/h4-8H,1-3H3
InchiKey: GFQUBQQRVARIRW-UHFFFAOYSA-N
Formula: C12H14
SMILES: CC1=CC(C)(C)c2ccccc21
Mol. weight [g/mol]: 158.24
CAS: 2177-45-9

Physical Properties

Property code	Value	Unit	Source
gf	228.53	kJ/mol	Joback Method
hf	68.40	kJ/mol	Joback Method
hfus	13.16	kJ/mol	Joback Method
hvap	44.96	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.381		Crippen Method
mcvol	141.020	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	516.74	K	Joback Method
tc	745.84	K	Joback Method
tf	319.06	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.01	J/mol×K	516.74	Joback Method
cpg	330.83	J/mol×K	554.92	Joback Method
cpg	345.43	J/mol×K	593.11	Joback Method
cpg	358.97	J/mol×K	631.29	Joback Method
cpg	371.63	J/mol×K	669.47	Joback Method
cpg	383.58	J/mol×K	707.65	Joback Method
cpg	394.98	J/mol×K	745.84	Joback Method

Sources

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=C2177459&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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