2,3,7,7-tetramethylcyclohepta-1,3,5-triene

Inchi: InChI=1S/C11H16/c1-9-6-5-7-11(3,4)8-10(9)2/h5-8H,1-4H3
InchiKey: QPLKPIRCFUUDGB-UHFFFAOYSA-N
Formula: C11H16
SMILES: CC1=CC=CC(C)(C)C=C1C
Mol. weight [g/mol]: 148.24

Physical Properties

Property code	Value	Unit	Source
gf	119.22	kJ/mol	Joback Method
hf	-56.57	kJ/mol	Joback Method
hfus	10.57	kJ/mol	Joback Method
hvap	41.73	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.475		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	1040.00		NIST Webbook
tb	482.58	K	Joback Method
tc	702.60	K	Joback Method
tf	268.81	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.62	J/mol×K	482.58	Joback Method
cpg	318.72	J/mol×K	519.25	Joback Method
cpg	334.71	J/mol×K	555.92	Joback Method
cpg	349.72	J/mol×K	592.59	Joback Method
cpg	363.84	J/mol×K	629.26	Joback Method
cpg	377.18	J/mol×K	665.93	Joback Method
cpg	389.85	J/mol×K	702.60	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=R492094&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume