1,5,5-trimethylcyclohepta-1,3-diene

Inchi: InChI=1S/C10H16/c1-9-5-4-7-10(2,3)8-6-9/h4-5,7H,6,8H2,1-3H3
InchiKey: ZEIJNNOODJKIOD-UHFFFAOYSA-N
Formula: C10H16
SMILES: CC1=CC=CC(C)(C)CC1
Mol. weight [g/mol]: 136.23

Physical Properties

Property code	Value	Unit	Source
gf	90.47	kJ/mol	Joback Method
hf	-82.24	kJ/mol	Joback Method
hfus	7.15	kJ/mol	Joback Method
hvap	38.55	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
rinpol	976.50		NIST Webbook
rinpol	976.50		NIST Webbook
tb	455.56	K	Joback Method
tc	675.30	K	Joback Method
tf	244.26	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.99	J/mol×K	455.56	Joback Method
cpg	290.03	J/mol×K	492.18	Joback Method
cpg	306.86	J/mol×K	528.81	Joback Method
cpg	322.59	J/mol×K	565.43	Joback Method
cpg	337.33	J/mol×K	602.05	Joback Method
cpg	351.19	J/mol×K	638.68	Joback Method
cpg	364.28	J/mol×K	675.30	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=R492074&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume