2,2,6-Trimethyl-hepta-3,5-diene

Inchi: InChI=1S/C10H18/c1-9(2)7-6-8-10(3,4)5/h6-8H,1-5H3/b8-6+
InchiKey: HRPDOMKMPKLUAK-SOFGYWHQSA-N
Formula: C10H18
SMILES: CC(C)=CC=CC(C)(C)C
Mol. weight [g/mol]: 138.25

Physical Properties

Property code	Value	Unit	Source
gf	188.05	kJ/mol	Joback Method
hf	-33.83	kJ/mol	Joback Method
hfus	13.34	kJ/mol	Joback Method
hvap	36.55	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.555		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1161.00		NIST Webbook
tb	433.17	K	Joback Method
tc	627.01	K	Joback Method
tf	180.76	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.98	J/mol×K	433.17	Joback Method
cpg	303.54	J/mol×K	465.48	Joback Method
cpg	319.10	J/mol×K	497.78	Joback Method
cpg	333.72	J/mol×K	530.09	Joback Method
cpg	347.47	J/mol×K	562.40	Joback Method
cpg	360.38	J/mol×K	594.70	Joback Method
cpg	372.53	J/mol×K	627.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R442014&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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