3,6,6-trimethylcycloheptene

Inchi: InChI=1S/C10H18/c1-9-5-4-7-10(2,3)8-6-9/h4-5,9H,6-8H2,1-3H3
InchiKey: YCTPMOKNQNWVDT-UHFFFAOYSA-N
Formula: C10H18
SMILES: CC1C=CCC(C)(C)CC1
Mol. weight [g/mol]: 138.25

Physical Properties

Property code	Value	Unit	Source
gf	62.43	kJ/mol	Joback Method
hf	-148.89	kJ/mol	Joback Method
hfus	7.39	kJ/mol	Joback Method
hvap	37.29	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.389		Crippen Method
mcvol	136.600	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	953.00		NIST Webbook
rinpol	953.00		NIST Webbook
tb	446.75	K	Joback Method
tc	662.46	K	Joback Method
tf	226.74	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.55	J/mol×K	446.75	Joback Method
cpg	305.78	J/mol×K	482.70	Joback Method
cpg	324.73	J/mol×K	518.65	Joback Method
cpg	342.50	J/mol×K	554.61	Joback Method
cpg	359.18	J/mol×K	590.56	Joback Method
cpg	374.89	J/mol×K	626.51	Joback Method
cpg	389.72	J/mol×K	662.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492138&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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