1,1,4-trimethylcycloheptene

Other names: 1,4,4-trimethylcycloheptene
Inchi: InChI=1S/C10H18/c1-9-5-4-7-10(2,3)8-6-9/h6H,4-5,7-8H2,1-3H3
InchiKey: CPKYAUHXXUMQDM-UHFFFAOYSA-N
Formula: C10H18
SMILES: CC1=CCC(C)(C)CCC1
Mol. weight [g/mol]: 138.25

Physical Properties

Property code	Value	Unit	Source
gf	60.51	kJ/mol	Joback Method
hf	-140.02	kJ/mol	Joback Method
hfus	5.93	kJ/mol	Joback Method
hvap	38.26	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.533		Crippen Method
mcvol	136.600	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	959.00		NIST Webbook
rinpol	959.00		NIST Webbook
tb	456.40	K	Joback Method
tc	673.85	K	Joback Method
tf	243.50	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.14	J/mol×K	456.40	Joback Method
cpg	306.46	J/mol×K	492.64	Joback Method
cpg	324.55	J/mol×K	528.88	Joback Method
cpg	341.51	J/mol×K	565.12	Joback Method
cpg	357.45	J/mol×K	601.37	Joback Method
cpg	372.47	J/mol×K	637.61	Joback Method
cpg	386.67	J/mol×K	673.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492014&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