1,2,5,5-tetramethylcycloheptene

Inchi: InChI=1S/C11H20/c1-9-5-7-11(3,4)8-6-10(9)2/h5-8H2,1-4H3
InchiKey: VXANAVFWLBEGSZ-UHFFFAOYSA-N
Formula: C11H20
SMILES: CC1=C(C)CCC(C)(C)CC1
Mol. weight [g/mol]: 152.28

Physical Properties

Property code	Value	Unit	Source
gf	59.30	kJ/mol	Joback Method
hf	-172.13	kJ/mol	Joback Method
hfus	8.13	kJ/mol	Joback Method
hvap	41.15	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.923		Crippen Method
mcvol	150.690	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1069.00		NIST Webbook
tb	484.26	K	Joback Method
tc	699.81	K	Joback Method
tf	267.29	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.19	J/mol×K	484.26	Joback Method
cpg	353.77	J/mol×K	520.19	Joback Method
cpg	372.21	J/mol×K	556.11	Joback Method
cpg	389.59	J/mol×K	592.04	Joback Method
cpg	406.01	J/mol×K	627.96	Joback Method
cpg	421.58	J/mol×K	663.89	Joback Method
cpg	436.39	J/mol×K	699.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492034&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