4,4-dimethyl-1,2-dimethylenecycloheptane

Inchi: InChI=1S/C11H18/c1-9-6-5-7-11(3,4)8-10(9)2/h1-2,5-8H2,3-4H3
InchiKey: XKVJKEYRYFLMLG-UHFFFAOYSA-N
Formula: C11H18
SMILES: C=C1CCCC(C)(C)CC1=C
Mol. weight [g/mol]: 150.26

Physical Properties

Property code	Value	Unit	Source
gf	154.76	kJ/mol	Joback Method
hf	-38.49	kJ/mol	Joback Method
hfus	5.37	kJ/mol	Joback Method
hvap	39.85	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.699		Crippen Method
mcvol	146.390	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1054.50		NIST Webbook
tb	473.46	K	Joback Method
tc	688.17	K	Joback Method
tf	268.85	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.01	J/mol×K	473.46	Joback Method
cpg	333.75	J/mol×K	509.25	Joback Method
cpg	351.36	J/mol×K	545.03	Joback Method
cpg	367.94	J/mol×K	580.82	Joback Method
cpg	383.59	J/mol×K	616.60	Joback Method
cpg	398.39	J/mol×K	652.39	Joback Method
cpg	412.44	J/mol×K	688.17	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=R492143&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