2,5,5-trimethyl-1-methylenecycloheptane

Inchi: InChI=1S/C11H20/c1-9-5-7-11(3,4)8-6-10(9)2/h10H,1,5-8H2,2-4H3
InchiKey: ZCXZRIYUMPKXQW-UHFFFAOYSA-N
Formula: C11H20
SMILES: C=C1CCC(C)(C)CCC1C
Mol. weight [g/mol]: 152.28

Physical Properties

Property code	Value	Unit	Source
gf	93.97	kJ/mol	Joback Method
hf	-143.07	kJ/mol	Joback Method
hfus	7.59	kJ/mol	Joback Method
hvap	39.38	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.779		Crippen Method
mcvol	150.690	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1031.00		NIST Webbook
tb	469.63	K	Joback Method
tc	682.11	K	Joback Method
tf	250.93	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.27	J/mol×K	469.63	Joback Method
cpg	351.91	J/mol×K	505.04	Joback Method
cpg	371.35	J/mol×K	540.46	Joback Method
cpg	389.68	J/mol×K	575.87	Joback Method
cpg	406.99	J/mol×K	611.28	Joback Method
cpg	423.37	J/mol×K	646.69	Joback Method
cpg	438.91	J/mol×K	682.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492103&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