1,1,3,3,5-Pentamethylcyclohexane

Inchi: InChI=1S/C11H22/c1-9-6-10(2,3)8-11(4,5)7-9/h9H,6-8H2,1-5H3
InchiKey: AUBOCPGIGWSTNB-UHFFFAOYSA-N
Formula: C11H22
SMILES: CC1CC(C)(C)CC(C)(C)C1
Mol. weight [g/mol]: 154.29
CAS: 70810-19-4

Physical Properties

Property code	Value	Unit	Source
gf	39.79	kJ/mol	Joback Method
hf	-226.25	kJ/mol	Joback Method
hfus	5.63	kJ/mol	Joback Method
hvap	37.59	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.859		Crippen Method
mcvol	154.990	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
tb	440.10 ± 3.00	K	NIST Webbook
tc	672.94	K	Joback Method
tf	260.43	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.58	J/mol×K	461.77	Joback Method
cpg	369.39	J/mol×K	496.97	Joback Method
cpg	389.67	J/mol×K	532.16	Joback Method
cpg	408.62	J/mol×K	567.36	Joback Method
cpg	426.40	J/mol×K	602.55	Joback Method
cpg	443.18	J/mol×K	637.75	Joback Method
cpg	459.14	J/mol×K	672.94	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=C70810194&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume