1-Ethyl-2,2,6-trimethylcyclohexane

Inchi: InChI=1S/C11H22/c1-5-10-9(2)7-6-8-11(10,3)4/h9-10H,5-8H2,1-4H3
InchiKey: WBGMHYJBJYDLTE-UHFFFAOYSA-N
Formula: C11H22
SMILES: CCC1C(C)CCCC1(C)C
Mol. weight [g/mol]: 154.29
CAS: 71186-27-1

Physical Properties

Property code	Value	Unit	Source
gf	45.28	kJ/mol	Joback Method
hf	-241.49	kJ/mol	Joback Method
hfus	11.92	kJ/mol	Joback Method
hvap	38.74	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.859		Crippen Method
mcvol	154.990	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
tb	461.53	K	Joback Method
tc	663.80	K	Joback Method
tf	236.53	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.84	J/mol×K	461.53	Joback Method
cpg	368.21	J/mol×K	495.24	Joback Method
cpg	388.38	J/mol×K	528.95	Joback Method
cpg	407.44	J/mol×K	562.67	Joback Method
cpg	425.47	J/mol×K	596.38	Joback Method
cpg	442.56	J/mol×K	630.09	Joback Method
cpg	458.80	J/mol×K	663.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71186271&Units=SI

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