Tricyclo[4.3.1.1(3,8)]undecane

Other names: Homoadamantane
Inchi: InChI=1S/C11H18/c1-2-9-5-10-3-8(1)4-11(6-9)7-10/h8-11H,1-7H2
InchiKey: LFWQUGCYGMCTQW-UHFFFAOYSA-N
Formula: C11H18
SMILES: C1CC2CC3CC1CC(C2)C3
Mol. weight [g/mol]: 150.26
CAS: 281-46-9

Physical Properties

Property code	Value	Unit	Source
gf	192.08	kJ/mol	Joback Method
hf	-84.63	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	39.85	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.223		Crippen Method
mcvol	133.270	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1235.20		NIST Webbook
rinpol	1235.20		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1255.00		NIST Webbook
tb	475.17	K	Joback Method
tc	694.16	K	Joback Method
tf	256.27	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.54	J/mol×K	475.17	Joback Method
cpg	342.32	J/mol×K	511.67	Joback Method

cpg	363.54	J/mol×K	548.17	Joback Method
cpg	383.31	J/mol×K	584.66	Joback Method
cpg	401.73	J/mol×K	621.16	Joback Method
cpg	418.89	J/mol×K	657.66	Joback Method
cpg	434.88	J/mol×K	694.16	Joback Method
dvisc	0.0010505	Pa×s	256.27	Joback Method
dvisc	0.0010619	Pa×s	292.75	Joback Method
dvisc	0.0010709	Pa×s	329.24	Joback Method
dvisc	0.0010782	Pa×s	365.72	Joback Method
dvisc	0.0010841	Pa×s	402.20	Joback Method
dvisc	0.0010891	Pa×s	438.69	Joback Method
dvisc	0.0010934	Pa×s	475.17	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C281469&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
dvisc: Dynamic viscosity
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