Bicyclo[3.3.3]undecane

Inchi: InChI=1S/C11H20/c1-4-10-6-2-7-11(5-1)9-3-8-10/h10-11H,1-9H2
InchiKey: NAVGAEZCCRCJQT-UHFFFAOYSA-N
Formula: C11H20
SMILES: C1CC2CCCC(C1)CCC2
Mol. weight [g/mol]: 152.28
CAS: 29415-95-0

Physical Properties

Property code	Value	Unit	Source
chs	-7034.00 ± 2.00	kJ/mol	NIST Webbook
gf	102.74	kJ/mol	Joback Method
hf	-89.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-152.50 ± 1.80	kJ/mol	NIST Webbook
hfus	10.02	kJ/mol	Joback Method
hsub	63.60 ± 0.84	kJ/mol	NIST Webbook
hsub	63.50	kJ/mol	NIST Webbook
hvap	40.77	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.757		Crippen Method
mcvol	144.130	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	485.91	K	Joback Method
tc	713.20	K	Joback Method
tf	232.01	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.24	J/mol×K	485.91	Joback Method
cpg	441.37	J/mol×K	675.32	Joback Method
cpg	422.69	J/mol×K	637.44	Joback Method
cpg	402.70	J/mol×K	599.56	Joback Method
cpg	381.33	J/mol×K	561.67	Joback Method

cpg	358.53	J/mol×K	523.79	Joback Method
cpg	458.77	J/mol×K	713.20	Joback Method
cps	213.20	J/mol×K	298.15	NIST Webbook
dvisc	0.0074291	Pa×s	232.01	Joback Method
dvisc	0.0003310	Pa×s	485.91	Joback Method
dvisc	0.0004341	Pa×s	443.59	Joback Method
dvisc	0.0006029	Pa×s	401.28	Joback Method
dvisc	0.0009046	Pa×s	358.96	Joback Method
dvisc	0.0015129	Pa×s	316.64	Joback Method
dvisc	0.0029653	Pa×s	274.33	Joback Method
hsubt	6.36	kJ/mol	298.15	NIST Webbook
ssubt	21.33	J/mol×K	298.15	NIST Webbook

Sources

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=C29415950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

ssubt:	Entropy of sublimation at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume