

Tricyclo[4.3.2.0(1,6)undeca-3-ene

Inchi:	InChI=1S/C11H16/c1-2-5-11-7-3-6-10(11,4-1)8-9-11/h1-2H,3-9H2
InchiKey:	AEVSDMKEZBQELO-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	C1=CCC23CCCC2(C1)CC3
Mol. weight [g/mol]:	148.24
CAS:	136630-09-6

Physical Properties

Property code	Value	Unit	Source
gf	226.48	kJ/mol	Joback Method
hf	44.31	kJ/mol	Joback Method
hfus	2.01	kJ/mol	Joback Method
hvap	38.46	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.287		Crippen Method
mcvol	128.970	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	484.15	K	Joback Method
tc	726.41	K	Joback Method
tf	313.31	K	Joback Method
vc	0.489	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.25	J/mol×K	484.15	Joback Method
cpg	325.24	J/mol×K	524.53	Joback Method
cpg	343.94	J/mol×K	564.90	Joback Method
cpg	360.76	J/mol×K	605.28	Joback Method
cpg	376.09	J/mol×K	645.66	Joback Method
cpg	390.30	J/mol×K	686.04	Joback Method
cpg	403.79	J/mol×K	726.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C136630096&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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