

Tricyclo[4.2.2.2(2,5)]dodec-3-ene

Inchi: InChI=1S/C12H18/c1-2-10-4-3-9(1)11-5-7-12(10)8-6-11/h1-2,9-12H,3-8H2
InchiKey: HEGVALGWBKXHA-UHFFFAOYSA-N
Formula: C12H18
SMILES: C1=CC2CCC1C1CCC2CC1
Mol. weight [g/mol]: 162.27
CAS: 69122-74-3

Physical Properties

Property code	Value	Unit	Source
gf	218.36	kJ/mol	Joback Method
hf	33.00	kJ/mol	NIST Webbook
hfus	17.23	kJ/mol	Joback Method
hvap	42.54	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.389		Crippen Method
mcvol	143.060	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	501.48	K	Joback Method
tc	727.69	K	Joback Method
tf	264.78	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.06	J/molxK	501.48	Joback Method
cpg	375.27	J/molxK	539.18	Joback Method
cpg	396.85	J/molxK	576.88	Joback Method
cpg	416.91	J/molxK	614.58	Joback Method
cpg	435.54	J/molxK	652.28	Joback Method
cpg	452.86	J/molxK	689.99	Joback Method
cpg	468.96	J/molxK	727.69	Joback Method
dvisc	0.0013809	Paxs	264.78	Joback Method
dvisc	0.0012585	Paxs	304.23	Joback Method

dvisc	0.0011717	Paxs	343.68	Joback Method
dvisc	0.0011070	Paxs	383.13	Joback Method
dvisc	0.0010571	Paxs	422.58	Joback Method
dvisc	0.0010173	Paxs	462.03	Joback Method
dvisc	0.0009850	Paxs	501.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69122743&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
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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