

Traginone=4-(6-methylbicyclo[4.1.0]hept-2-en-7-y

Other names:	Traginone
Inchi:	InChI=1S/C12H18O/c1-9(13)6-7-11-10-5-3-4-8-12(10,11)2/h3,5,10-11H,4,6-8H2,1-2H3
InchiKey:	RWTVZLVKCBKII-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CC(=O)CCC1C2C=CCCC21C
Mol. weight [g/mol]:	178.27

Physical Properties

Property code	Value	Unit	Source
gf	47.40	kJ/mol	Joback Method
hf	-211.47	kJ/mol	Joback Method
hfus	18.60	kJ/mol	Joback Method
hvap	47.88	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.958		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
ripol	1881.00		NIST Webbook
ripol	1881.00		NIST Webbook
ripol	1881.00		NIST Webbook
ripol	1881.00		NIST Webbook
tb	540.31	K	Joback Method
tc	751.97	K	Joback Method
tf	327.71	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.75	J/molxK	540.31	Joback Method
cpg	409.62	J/molxK	575.59	Joback Method
cpg	426.26	J/molxK	610.86	Joback Method
cpg	441.83	J/molxK	646.14	Joback Method
cpg	456.47	J/molxK	681.42	Joback Method

cpg	470.32	J/mol×K	716.70	Joback Method
cpg	483.55	J/mol×K	751.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418378&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
hvac:	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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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