

Bicyclo[2.2.1]heptan-2-one, 5,5,6-trimethyl-, endo-

Inchi:	InChI=1S/C10H16O/c1-6-8-4-7(5-9(8)11)10(6,2)3/h6-8H,4-5H2,1-3H3
InchiKey:	TZAXGXBLCOILBQ-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1C2CC(CC2=O)C1(C)C
Mol. weight [g/mol]:	152.23
CAS:	3767-44-0

Physical Properties

Property code	Value	Unit	Source
gf	-0.78	kJ/mol	Joback Method
hf	-273.43	kJ/mol	Joback Method
hfus	11.18	kJ/mol	Joback Method
hvap	40.33	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.258		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1165.00		NIST Webbook
tb	504.67	K	Joback Method
tc	727.60	K	Joback Method
tf	318.46	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.94	J/mol×K	504.67	Joback Method
cpg	343.76	J/mol×K	541.83	Joback Method
cpg	361.40	J/mol×K	578.98	Joback Method
cpg	377.96	J/mol×K	616.14	Joback Method
cpg	393.57	J/mol×K	653.29	Joback Method
cpg	408.36	J/mol×K	690.45	Joback Method
cpg	422.45	J/mol×K	727.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3767440&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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