[1S]-4,6,6-Trimethyl-bicyclo[3,1,1]hept-3-en-2-one

Inchi: InChI=1S/C9H12O/c1-9(2)6-3-4-8(10)7(9)5-6/h3-4,6-7H,5H2,1-2H3/t6-,7-/m0/s1
InchiKey: NNPXUZFTLBPVNP-BQBZGAKWSA-N
Formula: C9H12O
SMILES: CC1(C)C2C=CC(=O)C1C2
Mol. weight [g/mol]: 136.19

Physical Properties

Property code	Value	Unit	Source
gf	28.47	kJ/mol	Joback Method
hf	-174.67	kJ/mol	Joback Method
hfus	8.74	kJ/mol	Joback Method
hvap	38.70	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.788		Crippen Method
mcvol	113.220	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	1214.00		NIST Webbook
rinpol	1215.60		NIST Webbook
rinpol	1211.10		NIST Webbook
tb	485.62	K	Joback Method
tc	714.95	K	Joback Method
tf	312.19	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.17	J/mol×K	485.62	Joback Method
cpg	278.49	J/mol×K	523.84	Joback Method
cpg	293.61	J/mol×K	562.06	Joback Method
cpg	307.67	J/mol×K	600.28	Joback Method
cpg	320.82	J/mol×K	638.50	Joback Method
cpg	333.19	J/mol×K	676.73	Joback Method
cpg	344.93	J/mol×K	714.95	Joback Method

Sources

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=R419435&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume