trans-Bicyclo[3.3.0]-octan-2-one

Inchi: InChI=1S/C8H12O/c9-8-5-4-6-2-1-3-7(6)8/h6-7H,1-5H2/t6-,7+/m1/s1
InchiKey: NZTVVUIIJPWANB-RQJHMYQMSA-N
Formula: C8H12O
SMILES: O=C1CCC2CCCC12
Mol. weight [g/mol]: 124.18
CAS: 29365-79-5

Physical Properties

Property code	Value	Unit	Source
chl	-4602.80 ± 4.60	kJ/mol	NIST Webbook
gf	-8.81	kJ/mol	Joback Method
hf	-207.00 ± 5.40	kJ/mol	NIST Webbook
hfl	-260.00 ± 4.60	kJ/mol	NIST Webbook
hfus	8.06	kJ/mol	Joback Method
hvap	54.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-1.76		Crippen Method
logp	1.766		Crippen Method
mcvol	103.430	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	472.28	K	Joback Method
tc	702.14	K	Joback Method
tf	276.98	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.73	J/mol×K	472.28	Joback Method
cpg	250.02	J/mol×K	510.59	Joback Method
cpg	266.30	J/mol×K	548.90	Joback Method
cpg	281.60	J/mol×K	587.21	Joback Method
cpg	295.95	J/mol×K	625.52	Joback Method
cpg	309.40	J/mol×K	663.83	Joback Method
cpg	321.98	J/mol×K	702.14	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29365795&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume