2-Butanone, 4-(2,2,6-trimethylcyclohexyl)-

Other names: 4-(2,2,6-Trimethylcyclohexyl)-2-butanone
4-(2,6,6-trimethylcyclohexyl)butan-2-one
Inchi: InChI=1S/C13H24O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h10,12H,5-9H2,1-4H3
InchiKey: PQCDGQHNORPNBR-UHFFFAOYSA-N
Formula: C13H24O
SMILES: CC(=O)CCC1C(C)CCCC1(C)C
Mol. weight [g/mol]: 196.33
CAS: 6138-85-8

Physical Properties

Property code	Value	Unit	Source
gf	-66.80	kJ/mol	Joback Method
hf	-395.35	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	49.94	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.818		Crippen Method
mcvol	184.740	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
tb	561.16	K	Joback Method
tc	766.91	K	Joback Method
tf	309.00	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.29	J/mol×K	561.16	Joback Method
cpg	498.16	J/mol×K	595.45	Joback Method
cpg	517.90	J/mol×K	629.74	Joback Method
cpg	536.62	J/mol×K	664.03	Joback Method
cpg	554.39	J/mol×K	698.33	Joback Method

cpg	571.32	J/mol×K	732.62	Joback Method
cpg	587.49	J/mol×K	766.91	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=C6138858&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
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