Cyclohexanebutanal, 2-methyl-3-oxo-, cis-

Other names: 4-(2-Methyl-3-oxocyclohexyl)butanal
Inchi: InChI=1S/C11H18O2/c1-9-10(5-2-3-8-12)6-4-7-11(9)13/h8-10H,2-7H2,1H3/t9-,10-/m0/s1
InchiKey: NQONHVHHNWFPMU-UWVGGRQHSA-N
Formula: C11H18O2
SMILES: CC1C(=O)CCCC1CCCC=O
Mol. weight [g/mol]: 182.26
CAS: 92485-93-3

Physical Properties

Property code	Value	Unit	Source
gf	-163.63	kJ/mol	Joback Method
hf	-459.67	kJ/mol	Joback Method
hfus	18.95	kJ/mol	Joback Method
hvap	51.17	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.361		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1521.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1509.00		NIST Webbook
tb	582.44	K	Joback Method
tc	795.55	K	Joback Method
tf	327.09	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.50	J/mol×K	582.44	Joback Method
cpg	431.84	J/mol×K	617.96	Joback Method
cpg	449.23	J/mol×K	653.48	Joback Method
cpg	465.68	J/mol×K	688.99	Joback Method
cpg	481.16	J/mol×K	724.51	Joback Method

cpg	495.69	J/mol×K	760.03	Joback Method
cpg	509.26	J/mol×K	795.55	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=C92485933&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