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-/m1/s1
InchiKey: NQONHVHHNWFPMU-UWVGGRQHSA-N
Formula: C11H18O2
SMILES: C[C@H]1C(=O)CCC[C@H]1CCCC=O
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
hfus	18.95	kJ/mol	Joback Method
logp	2.361		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
rinpol	1509.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1509.00		NIST Webbook

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C92485933&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices