4-(2,2-Dimethyl-6-methylenecyclohexyl)butanal

Inchi: InChI=1S/C13H22O/c1-11-7-6-9-13(2,3)12(11)8-4-5-10-14/h10,12H,1,4-9H2,2-3H3
InchiKey: LEXVMOJLXLEPJE-UHFFFAOYSA-N
Formula: C13H22O
SMILES: C=C1CCCC(C)(C)C1CCCC=O
Mol. weight [g/mol]: 194.31
CAS: 95452-13-4

Physical Properties

Property code	Value	Unit	Source
gf	23.39	kJ/mol	Joback Method
hf	-263.77	kJ/mol	Joback Method
hfus	17.16	kJ/mol	Joback Method
hvap	50.38	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.738		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1703.00		NIST Webbook
tb	559.78	K	Joback Method
tc	762.61	K	Joback Method
tf	318.99	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.24	J/mol×K	559.78	Joback Method
cpg	475.07	J/mol×K	593.58	Joback Method
cpg	492.88	J/mol×K	627.39	Joback Method
cpg	509.76	J/mol×K	661.19	Joback Method
cpg	525.81	J/mol×K	695.00	Joback Method
cpg	541.11	J/mol×K	728.80	Joback Method
cpg	555.76	J/mol×K	762.61	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=C95452134&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

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