

3-Cyclohexene-1-carboxaldehyde, 3-(4-methyl-3-pentenyl)-

Other names:

Myrac aldehyde 1

3-Cyclohexene-1-carboxaldehyde, 3-(4-methyl-3-penten-1-yl)-

1-Formyl-3-(3-isohexenyl)-3-cyclohexene

m-Myrac aldehyde

3-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde

Inchi: InChI=1S/C13H20O/c1-11(2)5-3-6-12-7-4-8-13(9-12)10-14/h5,7,10,13H,3-4,6,8-9H2,1-2H

InchiKey: RKXHUEKKGCBVSR-UHFFFAOYSA-N

Formula: C13H20O

SMILES: CC(C)=CCCC1=CCCC(C=O)C1

Mol. weight [g/mol]: 192.30

CAS: 52475-89-5

Physical Properties

Property code	Value	Unit	Source
gf	75.51	kJ/mol	Joback Method
hf	-189.17	kJ/mol	Joback Method
hfus	23.28	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.658		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1490.80		NIST Webbook
tb	573.23	K	Joback Method
tc	781.91	K	Joback Method
tf	279.89	K	Joback Method
vc	0.680	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.64	J/mol×K	573.23	Joback Method
cpg	456.92	J/mol×K	608.01	Joback Method
cpg	474.14	J/mol×K	642.79	Joback Method

cpg	490.35	J/mol×K	677.57	Joback Method
cpg	505.60	J/mol×K	712.35	Joback Method
cpg	519.93	J/mol×K	747.13	Joback Method
cpg	533.39	J/mol×K	781.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52475895&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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