Lyral

Other names: 4-(4-hydroxy-4-methylpentyl)cyclohex-3-enecarbaldehyde
Inchi: InChI=1S/C13H22O2/c1-13(2,15)9-3-4-11-5-7-12(10-14)8-6-11/h5,10,12,15H,3-4,6-9H2,
InchiKey: ORMHZBNNECIKOH-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: CC(C)(O)CCCC1=CCC(C=O)CC1
Mol. weight [g/mol]: 210.31
CAS: 31906-04-4

Physical Properties

Property code	Value	Unit	Source
gf	-130.14	kJ/mol	Joback Method
hf	-457.58	kJ/mol	Joback Method
hfus	21.06	kJ/mol	Joback Method
hvap	68.02	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.853		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1690.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1692.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1661.00		NIST Webbook
tb	658.14	K	Joback Method
tc	853.70	K	Joback Method
tf	362.17	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	527.16	J/mol×K	658.14	Joback Method
cpg	542.88	J/mol×K	690.73	Joback Method
cpg	557.66	J/mol×K	723.33	Joback Method
cpg	571.55	J/mol×K	755.92	Joback Method
cpg	584.60	J/mol×K	788.51	Joback Method
cpg	596.84	J/mol×K	821.11	Joback Method
cpg	608.32	J/mol×K	853.70	Joback Method
dvisc	0.0057066	Pa×s	362.17	Joback Method
dvisc	0.0016967	Pa×s	411.50	Joback Method
dvisc	0.0006541	Pa×s	460.83	Joback Method
dvisc	0.0003032	Pa×s	510.15	Joback Method
dvisc	0.0001609	Pa×s	559.48	Joback Method
dvisc	0.0000947	Pa×s	608.81	Joback Method
dvisc	0.0000603	Pa×s	658.14	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31906044&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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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