2-Propenal, 3-(2,6,6-trimethyl-1-cyclohexen-1-yl)-

Other names: 3-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-propenal
2-Propenal, 3-(2,6,6-trimethylcyclohexen-1-yl)
3-(2,6,6-Trimethylcyclohexen-1-yl)-prop-2-enal
3-(2,6,6-trimethyl-1-cyclohexen-1-yl)acrylaldehyde

Inchi: InChI=1S/C12H18O/c1-10-6-4-8-12(2,3)11(10)7-5-9-13/h5,7,9H,4,6,8H2,1-3H3/b7-5+

InchiKey: FLOPAOUVAMIAJN-FNORWQNLSA-N

Formula: C12H18O

SMILES: CC1=C(C=CC=O)C(C)(C)CCC1

Mol. weight [g/mol]: 178.27

CAS: 4951-40-0

Physical Properties

Property code	Value	Unit	Source
gf	60.52	kJ/mol	Joback Method
hf	-154.97	kJ/mol	Joback Method
hfus	15.31	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.268		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1329.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1336.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1952.00		NIST Webbook
ripol	1952.00		NIST Webbook
tb	555.69	K	Joback Method
tc	773.51	K	Joback Method
tf	319.00	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.59	J/mol×K	555.69	Joback Method
cpg	405.48	J/mol×K	591.99	Joback Method
cpg	421.34	J/mol×K	628.30	Joback Method
cpg	436.28	J/mol×K	664.60	Joback Method
cpg	450.45	J/mol×K	700.90	Joback Method
cpg	463.95	J/mol×K	737.21	Joback Method
cpg	476.92	J/mol×K	773.51	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4951400&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume