(3E)-4-(2,3,6-trimethylphenyl)-3-buten-2-one

Other names: (E)-4-(2',3',6'-trimethylphenyl)-3-buten-2-one
Inchi: InChI=1S/C13H16O/c1-9-5-6-10(2)13(12(9)4)8-7-11(3)14/h5-8H,1-4H3/b8-7+
InchiKey: AHHGVKNOSDJAQN-BQYQJAHWSA-N
Formula: C13H16O
SMILES: CC(=O)C=Cc1c(C)ccc(C)c1C
Mol. weight [g/mol]: 188.27
CAS: 57461-21-9

Physical Properties

Property code	Value	Unit	Source
gf	93.40	kJ/mol	Joback Method
hf	-104.89	kJ/mol	Joback Method
hfus	24.10	kJ/mol	Joback Method
hvap	55.50	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.214		Crippen Method
mcvol	167.540	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
ripol	2102.00		NIST Webbook
tb	596.49	K	Joback Method
tc	813.26	K	Joback Method
tf	345.10	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.21	J/mol×K	596.49	Joback Method
cpg	462.60	J/mol×K	777.13	Joback Method
cpg	450.88	J/mol×K	741.00	Joback Method
cpg	438.41	J/mol×K	704.87	Joback Method
cpg	425.17	J/mol×K	668.75	Joback Method

cpg	411.12	J/mol×K	632.62	Joback Method
cpg	473.62	J/mol×K	813.26	Joback Method
dvisc	0.0001689	Pa×s	596.49	Joback Method
dvisc	0.0002078	Pa×s	554.59	Joback Method
dvisc	0.0002644	Pa×s	512.69	Joback Method
dvisc	0.0003513	Pa×s	470.80	Joback Method
dvisc	0.0004933	Pa×s	428.90	Joback Method
dvisc	0.0007457	Pa×s	387.00	Joback Method
dvisc	0.0012461	Pa×s	345.10	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=C57461219&Units=SI

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

Latest version available from: