

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

Inchi:	InChI=1S/C13H16O/c1-9-7-10(2)12(4)13(8-9)6-5-11(3)14/h5-8H,1-4H3/b6-5-
InchiKey:	UABKUEYIQHSUFJ-WAYWQWQTSA-N
Formula:	C13H16O
SMILES:	CC(=O)C=Cc1cc(C)cc(C)c1C
Mol. weight [g/mol]:	188.27

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
ripol	2290.00		NIST Webbook
ripol	2290.00		NIST Webbook
tb	596.49	K	Joback Method
tc	813.26	K	Joback Method
tf	345.10	K	Joback Method
vc	0.641	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.21	J/molxK	596.49	Joback Method
cpg	411.12	J/molxK	632.62	Joback Method
cpg	425.17	J/molxK	668.75	Joback Method
cpg	438.41	J/molxK	704.87	Joback Method
cpg	450.88	J/molxK	741.00	Joback Method
cpg	462.60	J/molxK	777.13	Joback Method
cpg	473.62	J/molxK	813.26	Joback Method
dvisc	0.0012461	Paxs	345.10	Joback Method

dvisc	0.0007457	Paxs	387.00	Joback Method
dvisc	0.0004933	Paxs	428.90	Joback Method
dvisc	0.0003513	Paxs	470.80	Joback Method
dvisc	0.0002644	Paxs	512.69	Joback Method
dvisc	0.0002078	Paxs	554.59	Joback Method
dvisc	0.0001689	Paxs	596.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R339205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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