1-(2,3,6-trimethylphenyl)-3-buten-2-one

Inchi: InChI=1S/C13H16O/c1-5-12(14)8-13-10(3)7-6-9(2)11(13)4/h5-7H,1,8H2,2-4H3
InchiKey: KBGDCKHDBZJUKE-UHFFFAOYSA-N
Formula: C13H16O
SMILES: C=CC(=O)Cc1c(C)ccc(C)c1C
Mol. weight [g/mol]: 188.27
CAS: 54789-45-6

Physical Properties

Property code	Value	Unit	Source
gf	101.02	kJ/mol	Joback Method
hf	-96.68	kJ/mol	Joback Method
hfus	22.62	kJ/mol	Joback Method
hvap	54.87	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.909		Crippen Method
mcvol	167.540	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
ripol	2180.00		NIST Webbook
tb	589.01	K	Joback Method
tc	801.05	K	Joback Method
tf	348.42	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.63	J/mol×K	589.01	Joback Method
cpg	461.76	J/mol×K	765.71	Joback Method
cpg	450.05	J/mol×K	730.37	Joback Method
cpg	437.61	J/mol×K	695.03	Joback Method
cpg	424.41	J/mol×K	659.69	Joback Method
cpg	410.42	J/mol×K	624.35	Joback Method
cpg	472.76	J/mol×K	801.05	Joback Method
dvisc	0.0002037	Pa×s	589.01	Joback Method

dvisc	0.0002483	Pa×s	548.91	Joback Method
dvisc	0.0003122	Pa×s	508.81	Joback Method
dvisc	0.0004082	Pa×s	468.72	Joback Method
dvisc	0.0005612	Pa×s	428.62	Joback Method
dvisc	0.0008240	Pa×s	388.52	Joback Method
dvisc	0.0013218	Pa×s	348.42	Joback Method

Sources

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=C54789456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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