2,6-(CH3)2C6H3-COCH3

Other names: 2,6-(CH3)2C6H3-COCH3
Inchi: InChI=1S/C10H12O/c1-7-5-4-6-8(2)10(7)9(3)11/h4-6H,1-3H3
InchiKey: DDXBCZCBZGPSHD-UHFFFAOYSA-N
Formula: C10H12O
SMILES: CC(=O)c1c(C)cccc1C
Mol. weight [g/mol]: 148.21

Physical Properties

Property code	Value	Unit	Source
af	0.4669		Cheméo Relay (1.0)
affp	857.00	kJ/mol	NIST Webbook
basg	825.20	kJ/mol	NIST Webbook
gf	-2.45	kJ/mol	Joback Method
hf	-156.32	kJ/mol	Cheméo Relay (1.0)
hfus	16.52	kJ/mol	Joback Method
hvap	57.13	kJ/mol	Cheméo Relay (1.0)
ie	8.84	eV	Cheméo Relay (1.0)
log10ws	-2.30		Cheméo Relay (1.0)
logp	2.506		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	499.52	K	Cheméo Relay (1.0)
tc	728.65	K	Cheméo Relay (1.0)
tf	293.92 ± 0.25	K	NIST Webbook
vc	0.468	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.59	J/mol×K	518.71	Joback Method
cpg	289.78	J/mol×K	554.92	Joback Method
cpg	302.26	J/mol×K	591.14	Joback Method
cpg	314.04	J/mol×K	627.35	Joback Method
cpg	325.13	J/mol×K	663.56	Joback Method

cpg	335.57	J/mol×K	699.77	Joback Method
cpg	345.38	J/mol×K	735.99	Joback Method
dvisc	0.0017002	Pa×s	303.85	Joback Method
dvisc	0.0010355	Pa×s	339.66	Joback Method
dvisc	0.0006932	Pa×s	375.47	Joback Method
dvisc	0.0004977	Pa×s	411.28	Joback Method
dvisc	0.0003768	Pa×s	447.09	Joback Method
dvisc	0.0002973	Pa×s	482.90	Joback Method
dvisc	0.0002423	Pa×s	518.71	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2142769&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
affp: Proton affinity
basg: Gas basicity
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume