Pentane-2,4-dione, 3-(4-methoxybenzoyl)-

Inchi: InChI=1S/C13H14O4/c1-8(14)12(9(2)15)13(16)10-4-6-11(17-3)7-5-10/h4-7,12H,1-3H3
InchiKey: CRQNKYNTSKUTDE-UHFFFAOYSA-N
Formula: C13H14O4
SMILES: COc1ccc(C(=O)C(C(C)=O)C(C)=O)cc1
Mol. weight [g/mol]: 234.25
CAS: 137833-36-4

Physical Properties

Property code	Value	Unit	Source
gf	-332.84	kJ/mol	Joback Method
hf	-561.83	kJ/mol	Joback Method
hfus	25.54	kJ/mol	Joback Method
hvap	69.73	kJ/mol	Joback Method
ie	7.86	eV	NIST Webbook
log10ws	-2.24		Crippen Method
logp	1.672		Crippen Method
mcvol	180.850	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
tb	712.09	K	Joback Method
tc	933.07	K	Joback Method
tf	432.23	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.39	J/mol×K	712.09	Joback Method
cpg	532.90	J/mol×K	896.24	Joback Method
cpg	523.60	J/mol×K	859.41	Joback Method
cpg	513.41	J/mol×K	822.58	Joback Method
cpg	502.33	J/mol×K	785.75	Joback Method
cpg	490.33	J/mol×K	748.92	Joback Method
cpg	541.35	J/mol×K	933.07	Joback Method
dvisc	0.0001594	Pa×s	712.09	Joback Method

dvisc	0.0002022	Pa×s	665.45	Joback Method
dvisc	0.0002658	Pa×s	618.80	Joback Method
dvisc	0.0003654	Pa×s	572.16	Joback Method
dvisc	0.0005315	Pa×s	525.52	Joback Method
dvisc	0.0008316	Pa×s	478.87	Joback Method
dvisc	0.0014331	Pa×s	432.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C137833364&Units=SI
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

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
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