1-(4-Carbomethoxyphenyl)-1,2-butanedione

Other names: 4 -methyl-«alpha»-pyrrolidinobutyrophenone-M (carboxy-desamino-oxo-) methyl
Inchi: InChI=1S/C12H12O4/c1-3-10(13)11(14)8-4-6-9(7-5-8)12(15)16-2/h4-7H,3H2,1-2H3
InchiKey: GIGJHMZMJPJVOR-UHFFFAOYSA-N
Formula: C12H12O4
SMILES: CCC(=O)C(=O)c1ccc(C(=O)OC)cc1
Mol. weight [g/mol]: 220.22

Physical Properties

Property code	Value	Unit	Source
gf	-338.82	kJ/mol	Joback Method
hf	-535.91	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	67.89	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.635		Crippen Method
mcvol	166.760	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
tb	689.65	K	Joback Method
tc	910.24	K	Joback Method
tf	435.96	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.69	J/mol×K	689.65	Joback Method
cpg	437.84	J/mol×K	726.41	Joback Method
cpg	449.14	J/mol×K	763.18	Joback Method
cpg	459.59	J/mol×K	799.94	Joback Method
cpg	469.22	J/mol×K	836.71	Joback Method
cpg	478.04	J/mol×K	873.47	Joback Method
cpg	486.07	J/mol×K	910.24	Joback Method

dvisc	0.0013238	Pa×s	435.96	Joback Method
dvisc	0.0008332	Pa×s	478.24	Joback Method
dvisc	0.0005654	Pa×s	520.52	Joback Method
dvisc	0.0004066	Pa×s	562.81	Joback Method
dvisc	0.0003063	Pa×s	605.09	Joback Method
dvisc	0.0002394	Pa×s	647.37	Joback Method
dvisc	0.0001928	Pa×s	689.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360386&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume