2,4-Pentanedione, 3-(phenylmethyl)-

Other names: 2,4-Pentanedione, 3-benzyl-
3-Benzyl-2,4-pentanedione
Inchi: InChI=1S/C12H14O2/c1-9(13)12(10(2)14)8-11-6-4-3-5-7-11/h3-7,12H,8H2,1-2H3
InchiKey: WAJQTBOWJRUOOO-UHFFFAOYSA-N
Formula: C12H14O2
SMILES: CC(=O)C(Cc1ccccc1)C(C)=O
Mol. weight [g/mol]: 190.24
CAS: 1134-87-8

Physical Properties

Property code	Value	Unit	Source
gf	-97.71	kJ/mol	Joback Method
hf	-284.92	kJ/mol	Joback Method
hfus	20.55	kJ/mol	Joback Method
hvap	57.69	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.023		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
tb	607.94	K	Joback Method
tc	828.22	K	Joback Method
tf	336.28	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.83	J/mol×K	607.94	Joback Method
cpg	402.29	J/mol×K	644.65	Joback Method
cpg	415.78	J/mol×K	681.37	Joback Method
cpg	428.35	J/mol×K	718.08	Joback Method
cpg	440.03	J/mol×K	754.79	Joback Method
cpg	450.87	J/mol×K	791.50	Joback Method
cpg	460.91	J/mol×K	828.22	Joback Method

dvisc	0.0032069	Pa×s	336.28	Joback Method
dvisc	0.0015812	Pa×s	381.56	Joback Method
dvisc	0.0009058	Pa×s	426.83	Joback Method
dvisc	0.0005774	Pa×s	472.11	Joback Method
dvisc	0.0003983	Pa×s	517.39	Joback Method
dvisc	0.0002916	Pa×s	562.66	Joback Method
dvisc	0.0002237	Pa×s	607.94	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1134878&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume