Ethyl 2-benzylacetoacetate

Other names:	Ethyl «alpha»-benzylacetoacetate
	Ethyl benzylacetoacetate
	Benzenepropanoic acid, «alpha»-acetyl-, ethyl ester
	Ethyl «alpha»-acetylhydrocinnamate
	Ethyl 2-acetyl-3-phenylpropionate
	Hydrocinnamic acid, «alpha»-acetyl-, ethyl ester
	Ethyl 2-benzyl-3-oxobutanoate
	Ethyl-a-benzylacetoacetate
Inchi:	InChI=1S/C13H16O3/c1-3-16-13(15)12(10(2)14)9-11-7-5-4-6-8-11/h4-8,12H,3,9H2,1-2H
InchiKey:	XDWQYMXQMNUWID-UHFFFAOYSA-N
Formula:	C13H16O3
SMILES:	CCOC(=O)C(Cc1ccccc1)C(C)=O
Mol. weight [g/mol]:	220.26
CAS:	620-79-1

Physical Properties

Property code	Value	Unit	Source
gf	-194.29	kJ/mol	Joback Method
hf	-437.78	kJ/mol	Joback Method
hfus	24.33	kJ/mol	Joback Method
hvap	62.32	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.997		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
tb	549.20	K	NIST Webbook
tc	867.17	K	Joback Method
tf	369.78	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.09	J/mol×K	653.24	Joback Method

cpg	477.76	J/mol×K	688.89	Joback Method
cpg	491.50	J/mol×K	724.55	Joback Method
cpg	504.31	J/mol×K	760.20	Joback Method
cpg	516.23	J/mol×K	795.86	Joback Method
cpg	527.28	J/mol×K	831.51	Joback Method
cpg	537.49	J/mol×K	867.17	Joback Method
dvisc	0.0021636	Pa×s	369.78	Joback Method
dvisc	0.0010959	Pa×s	417.02	Joback Method
dvisc	0.0006375	Pa×s	464.27	Joback Method
dvisc	0.0004099	Pa×s	511.51	Joback Method
dvisc	0.0002840	Pa×s	558.75	Joback Method
dvisc	0.0002083	Pa×s	606.00	Joback Method
dvisc	0.0001598	Pa×s	653.24	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C620791&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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