Benzenepropanoic acid, «beta»-oxo-«alpha»-(phenylmethylene)-, ethyl ester

Inchi: InChI=1S/C18H16O3/c1-2-21-18(20)16(13-14-9-5-3-6-10-14)17(19)15-11-7-4-8-12-15/h3
InchiKey: BHKXLHNAIARBLO-DTQAZKPQSA-N
Formula: C18H16O3
SMILES: CCOC(=O)C(=Cc1ccccc1)C(=O)c1ccccc1
Mol. weight [g/mol]: 280.32
CAS: 17451-18-2

Physical Properties

Property code	Value	Unit	Source
gf	34.33	kJ/mol	Joback Method
hf	-191.74	kJ/mol	Joback Method
hfus	33.74	kJ/mol	Joback Method
hvap	76.15	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.516		Crippen Method
mcvol	221.670	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
tb	798.80	K	Joback Method
tc	1040.45	K	Joback Method
tf	448.51	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.40	J/mol×K	798.80	Joback Method
cpg	630.70	J/mol×K	839.08	Joback Method
cpg	643.79	J/mol×K	879.35	Joback Method
cpg	655.75	J/mol×K	919.63	Joback Method
cpg	666.67	J/mol×K	959.90	Joback Method
cpg	676.64	J/mol×K	1000.18	Joback Method
cpg	685.76	J/mol×K	1040.45	Joback Method

Sources

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=C17451182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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