Dibenzoylacetic acid, ethyl ester

Other names: ethyl 2-benzoyl-3-oxo-3-phenylpropionate
Inchi: InChI=1S/C18H16O4/c1-2-22-18(21)15(16(19)13-9-5-3-6-10-13)17(20)14-11-7-4-8-12-14
InchiKey: JHWPTSCKSATEQK-UHFFFAOYSA-N
Formula: C18H16O4
SMILES: CCOC(=O)C(C(=O)c1ccccc1)C(=O)c1ccccc1
Mol. weight [g/mol]: 296.32
CAS: 4850-82-2

Physical Properties

Property code	Value	Unit	Source
gf	-168.70	kJ/mol	Joback Method
hf	-417.03	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	82.47	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.931		Crippen Method
mcvol	227.540	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
tb	848.19	K	Joback Method
tc	1087.34	K	Joback Method
tf	502.48	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.94	J/mol×K	848.19	Joback Method
cpg	667.70	J/mol×K	888.05	Joback Method
cpg	679.20	J/mol×K	927.91	Joback Method
cpg	689.51	J/mol×K	967.77	Joback Method
cpg	698.68	J/mol×K	1007.63	Joback Method
cpg	706.79	J/mol×K	1047.48	Joback Method
cpg	713.90	J/mol×K	1087.34	Joback Method
dvisc	0.0009476	Pa×s	502.48	Joback Method

dvisc	0.0005158	Pa×s	560.10	Joback Method
dvisc	0.0003145	Pa×s	617.72	Joback Method
dvisc	0.0002087	Pa×s	675.34	Joback Method
dvisc	0.0001477	Pa×s	732.95	Joback Method
dvisc	0.0001099	Pa×s	790.57	Joback Method
dvisc	0.0000851	Pa×s	848.19	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=C4850822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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