O-benzoylbenzoic acid, ethyl ester

Other names: ethyl 2-(benzoyl)benzoate
Inchi: InChI=1S/C16H14O3/c1-2-19-16(18)14-11-7-6-10-13(14)15(17)12-8-4-3-5-9-12/h3-11H,2
InchiKey: CGWFVEFHQWJOKI-UHFFFAOYSA-N
Formula: C16H14O3
SMILES: CCOC(=O)c1ccccc1C(=O)c1ccccc1
Mol. weight [g/mol]: 254.28
CAS: 604-61-5

Physical Properties

Property code	Value	Unit	Source
gf	-63.81	kJ/mol	Joback Method
hf	-269.36	kJ/mol	Joback Method
hfus	29.28	kJ/mol	Joback Method
hvap	72.33	kJ/mol	Joback Method
log10ws	-3.40		Aqueous Solubility Prediction Method
logp	3.094		Crippen Method
mcvol	197.790	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
tb	753.98	K	Joback Method
tc	993.12	K	Joback Method
tf	332.65	K	Aqueous Solubility Prediction Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.75	J/mol×K	753.98	Joback Method
cpg	591.34	J/mol×K	953.26	Joback Method
cpg	581.82	J/mol×K	913.40	Joback Method
cpg	571.26	J/mol×K	873.55	Joback Method
cpg	559.59	J/mol×K	833.69	Joback Method
cpg	546.77	J/mol×K	793.84	Joback Method

cpg	599.86	J/mol×K	993.12	Joback Method
dvisc	0.0001229	Pa×s	753.98	Joback Method
dvisc	0.0001543	Pa×s	704.57	Joback Method
dvisc	0.0002005	Pa×s	655.16	Joback Method
dvisc	0.0002720	Pa×s	605.75	Joback Method
dvisc	0.0003893	Pa×s	556.35	Joback Method
dvisc	0.0005977	Pa×s	506.94	Joback Method
dvisc	0.0010066	Pa×s	457.53	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C604615&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