1,2-Ethanediol, dibenzoate

Other names:	Ethylene glycol, dibenzoate
	Benzoflex e-60
	Benzoflex 998
	Dibenzoyl ethylene glycol
	Ethylene dibenzoate
	Glycol dibenzoate
	Polyethylene-glycol (200) dibenzoate
	2-(Benzoyloxy)ethyl benzoate
Inchi:	InChI=1S/C16H14O4/c17-15(13-7-3-1-4-8-13)19-11-12-20-16(18)14-9-5-2-6-10-14/h1-10
InchiKey:	XFDQLDNQZFOAFK-UHFFFAOYSA-N
Formula:	C16H14O4
SMILES:	O=C(OCCOC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	270.28
CAS:	94-49-5

Physical Properties

Property code	Value	Unit	Source
gf	-159.18	kJ/mol	Joback Method
hf	-390.11	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	74.07	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	2.700		Crippen Method
mcvol	203.660	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	771.42	K	Joback Method
tc	1006.54	K	Joback Method
tf	467.24	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.80	J/mol×K	771.42	Joback Method
cpg	573.45	J/mol×K	810.61	Joback Method
cpg	585.87	J/mol×K	849.79	Joback Method
cpg	597.10	J/mol×K	888.98	Joback Method
cpg	607.18	J/mol×K	928.17	Joback Method
cpg	616.14	J/mol×K	967.36	Joback Method
cpg	624.01	J/mol×K	1006.54	Joback Method
dvisc	0.0008585	Pa×s	467.24	Joback Method
dvisc	0.0004959	Pa×s	517.94	Joback Method
dvisc	0.0003158	Pa×s	568.63	Joback Method
dvisc	0.0002166	Pa×s	619.33	Joback Method
dvisc	0.0001573	Pa×s	670.03	Joback Method
dvisc	0.0001194	Pa×s	720.72	Joback Method
dvisc	0.0000941	Pa×s	771.42	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=C94495&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

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