

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	Paxs	467.24	Joback Method
dvisc	0.0004959	Paxs	517.94	Joback Method
dvisc	0.0003158	Paxs	568.63	Joback Method
dvisc	0.0002166	Paxs	619.33	Joback Method
dvisc	0.0001573	Paxs	670.03	Joback Method
dvisc	0.0001194	Paxs	720.72	Joback Method
dvisc	0.0000941	Paxs	771.42	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=C94495&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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

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