1,3-Propanediol dibenzoate

Other names: Trimethyleneglycol, dibenzoate
Benzoflex S-432
TMETB
Inchi: InChI=1S/C17H16O4/c18-16(14-8-3-1-4-9-14)20-12-7-13-21-17(19)15-10-5-2-6-11-15/h1
InchiKey: SSEOOCRUUJYCKA-UHFFFAOYSA-N
Formula: C17H16O4
SMILES: O=C(OCCCOC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 284.31
CAS: 2451-86-7

Physical Properties

Property code	Value	Unit	Source
gf	-150.76	kJ/mol	Joback Method
hf	-410.75	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	76.30	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.090		Crippen Method
mcvol	217.750	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	2248.00		NIST Webbook
tb	794.30	K	Joback Method
tc	1025.52	K	Joback Method
tf	478.51	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.11	J/mol×K	794.30	Joback Method
cpg	628.00	J/mol×K	832.84	Joback Method
cpg	640.64	J/mol×K	871.37	Joback Method
cpg	652.08	J/mol×K	909.91	Joback Method
cpg	662.36	J/mol×K	948.45	Joback Method

cpg	671.52	J/mol×K	986.98	Joback Method
cpg	679.59	J/mol×K	1025.52	Joback Method
dvisc	0.0007896	Pa×s	478.51	Joback Method
dvisc	0.0004501	Pa×s	531.14	Joback Method
dvisc	0.0002839	Pa×s	583.77	Joback Method
dvisc	0.0001933	Pa×s	636.40	Joback Method
dvisc	0.0001395	Pa×s	689.04	Joback Method
dvisc	0.0001055	Pa×s	741.67	Joback Method
dvisc	0.0000828	Pa×s	794.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2451867&Units=SI
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

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