1,2-Benzenediol, O,O'-di(isobutoxycarbonyl)-

Other names: catechol, isoBOC
Inchi: InChI=1S/C16H22O6/c1-11(2)9-19-15(17)21-13-7-5-6-8-14(13)22-16(18)20-10-12(3)4/h5
InchiKey: NCKNEXUTRGASGF-UHFFFAOYSA-N
Formula: C16H22O6
SMILES: CC(C)COC(=O)Oc1ccccc1OC(=O)OCC(C)C
Mol. weight [g/mol]: 310.34

Physical Properties

Property code	Value	Unit	Source
gf	-496.10	kJ/mol	Joback Method
hf	-913.11	kJ/mol	Joback Method
hfus	31.75	kJ/mol	Joback Method
hvap	76.50	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	4.029		Crippen Method
mcvol	239.160	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	1961.00		NIST Webbook
tb	793.68	K	Joback Method
tc	999.55	K	Joback Method
tf	467.80	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.25	J/mol×K	793.68	Joback Method
cpg	719.96	J/mol×K	827.99	Joback Method
cpg	733.54	J/mol×K	862.30	Joback Method
cpg	745.96	J/mol×K	896.62	Joback Method
cpg	757.23	J/mol×K	930.93	Joback Method
cpg	767.32	J/mol×K	965.24	Joback Method
cpg	776.22	J/mol×K	999.55	Joback Method
dvisc	0.0005597	Pa×s	467.80	Joback Method

dvisc	0.0002966	Pa×s	522.11	Joback Method
dvisc	0.0001772	Pa×s	576.43	Joback Method
dvisc	0.0001156	Pa×s	630.74	Joback Method
dvisc	0.0000808	Pa×s	685.05	Joback Method
dvisc	0.0000595	Pa×s	739.37	Joback Method
dvisc	0.0000457	Pa×s	793.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U329732&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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