1,4-Butanediol, dibenzoate

Other names: 1,4-Butylene glycol dibenzoate
Benzoic acid, butylene ester
Inchi: InChI=1S/C18H18O4/c19-17(15-9-3-1-4-10-15)21-13-7-8-14-22-18(20)16-11-5-2-6-12-16
InchiKey: YHOWYTOWCBNTHB-UHFFFAOYSA-N
Formula: C18H18O4
SMILES: O=C(OCCCCOC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 298.33
CAS: 19224-27-2

Physical Properties

Property code	Value	Unit	Source
gf	-142.34	kJ/mol	Joback Method
hf	-431.39	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	78.53	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.481		Crippen Method
mcvol	231.840	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	2372.00		NIST Webbook
rinpol	2372.00		NIST Webbook
tb	817.18	K	Joback Method
tc	1045.05	K	Joback Method
tf	489.78	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.40	J/mol×K	817.18	Joback Method
cpg	683.46	J/mol×K	855.16	Joback Method
cpg	696.27	J/mol×K	893.14	Joback Method
cpg	707.87	J/mol×K	931.12	Joback Method
cpg	718.30	J/mol×K	969.10	Joback Method

cpg	727.60	J/mol×K	1007.08	Joback Method
cpg	735.82	J/mol×K	1045.05	Joback Method
dvisc	0.0007223	Pa×s	489.78	Joback Method
dvisc	0.0004065	Pa×s	544.35	Joback Method
dvisc	0.0002540	Pa×s	598.91	Joback Method
dvisc	0.0001717	Pa×s	653.48	Joback Method
dvisc	0.0001233	Pa×s	708.05	Joback Method
dvisc	0.0000928	Pa×s	762.61	Joback Method
dvisc	0.0000726	Pa×s	817.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19224272&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