1,3-Butanediol, dibenzoate

Inchi: InChI=1S/C18H18O4/c1-14(22-18(20)16-10-6-3-7-11-16)12-13-21-17(19)15-8-4-2-5-9-15
InchiKey: HVWZDMVPWXVEBP-UHFFFAOYSA-N
Formula: C18H18O4
SMILES: CC(CCOC(=O)c1ccccc1)OC(=O)c1ccccc1
Mol. weight [g/mol]: 298.33

Physical Properties

Property code	Value	Unit	Source
gf	-144.78	kJ/mol	Joback Method
hf	-436.67	kJ/mol	Joback Method
hfus	32.51	kJ/mol	Joback Method
hvap	78.14	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.479		Crippen Method
mcvol	231.840	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	2246.00		NIST Webbook
tb	816.74	K	Joback Method
tc	1048.22	K	Joback Method
tf	474.78	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.97	J/mol×K	816.74	Joback Method
cpg	728.71	J/mol×K	1009.64	Joback Method
cpg	719.40	J/mol×K	971.06	Joback Method
cpg	708.92	J/mol×K	932.48	Joback Method
cpg	697.21	J/mol×K	893.90	Joback Method
cpg	684.25	J/mol×K	855.32	Joback Method
cpg	736.89	J/mol×K	1048.22	Joback Method
dvisc	0.0000666	Pa×s	816.74	Joback Method
dvisc	0.0000865	Pa×s	759.75	Joback Method

dvisc	0.0001172	Pa×s	702.75	Joback Method
dvisc	0.0001676	Pa×s	645.76	Joback Method
dvisc	0.0002568	Pa×s	588.77	Joback Method
dvisc	0.0004312	Pa×s	531.77	Joback Method
dvisc	0.0008199	Pa×s	474.78	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=R322920&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