Glycerol dibenzoate

Inchi: InChI=1S/C17H16O5/c18-11-15(22-17(20)14-9-5-2-6-10-14)12-21-16(19)13-7-3-1-4-8-13
InchiKey: ZFSFYLDWVFNLFA-UHFFFAOYSA-N
Formula: C17H16O5
SMILES: O=C(OCC(CO)OC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 300.31

Physical Properties

Property code	Value	Unit	Source
gf	-290.02	kJ/mol	Joback Method
hf	-568.26	kJ/mol	Joback Method
hfus	34.01	kJ/mol	Joback Method
hvap	92.59	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.061		Crippen Method
mcvol	223.620	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	2442.00		NIST Webbook
rinpol	2442.00		NIST Webbook
tb	886.04	K	Joback Method
tc	1109.14	K	Joback Method
tf	524.33	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.19	J/mol×K	886.04	Joback Method
cpg	707.15	J/mol×K	1071.96	Joback Method
cpg	700.59	J/mol×K	1034.78	Joback Method
cpg	693.05	J/mol×K	997.59	Joback Method
cpg	684.50	J/mol×K	960.41	Joback Method
cpg	674.89	J/mol×K	923.22	Joback Method
cpg	712.77	J/mol×K	1109.14	Joback Method
dvisc	0.0000114	Pa×s	886.04	Joback Method

dvisc	0.0000164	Pa×s	825.75	Joback Method
dvisc	0.0000251	Pa×s	765.47	Joback Method
dvisc	0.0000414	Pa×s	705.18	Joback Method
dvisc	0.0000749	Pa×s	644.90	Joback Method
dvisc	0.0001532	Pa×s	584.62	Joback Method
dvisc	0.0003692	Pa×s	524.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R17949&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