Diglycolic acid, 4-bromophenyl heptyl ester

Inchi: InChI=1S/C17H23BrO5/c1-2-3-4-5-6-11-22-16(19)12-21-13-17(20)23-15-9-7-14(18)8-10-
InchiKey: CYAJDZFCEZGGKD-UHFFFAOYSA-N
Formula: C17H23BrO5
SMILES: CCCCCCCOC(=O)COCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 387.27

Physical Properties

Property code	Value	Unit	Source
gf	-363.48	kJ/mol	Joback Method
hf	-764.64	kJ/mol	Joback Method
hfus	45.48	kJ/mol	Joback Method
hvap	83.53	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.885		Crippen Method
mcvol	264.880	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	3152.00		NIST Webbook
rinpol	3152.00		NIST Webbook
tb	861.18	K	Joback Method
tc	1072.02	K	Joback Method
tf	546.64	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.32	J/mol×K	861.18	Joback Method
cpg	784.62	J/mol×K	896.32	Joback Method
cpg	796.80	J/mol×K	931.46	Joback Method
cpg	807.89	J/mol×K	966.60	Joback Method
cpg	817.89	J/mol×K	1001.74	Joback Method
cpg	826.81	J/mol×K	1036.88	Joback Method
cpg	834.66	J/mol×K	1072.02	Joback Method
dvisc	0.0003788	Pa×s	546.64	Joback Method

dvisc	0.0002329	Pa×s	599.06	Joback Method
dvisc	0.0001549	Pa×s	651.49	Joback Method
dvisc	0.0001095	Pa×s	703.91	Joback Method
dvisc	0.0000812	Pa×s	756.33	Joback Method
dvisc	0.0000626	Pa×s	808.76	Joback Method
dvisc	0.0000498	Pa×s	861.18	Joback Method

Sources

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=U381899&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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