Diglycolic acid, di(4-bromophenyl) ester

Inchi: InChI=1S/C16H12Br2O5/c17-11-1-5-13(6-2-11)22-15(19)9-21-10-16(20)23-14-7-3-12(18
InchiKey: TXHVJPLIBJHVLN-UHFFFAOYSA-N
Formula: C16H12Br2O5
SMILES: O=C(COCC(=O)Oc1ccc(Br)cc1)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 444.07

Physical Properties

Property code	Value	Unit	Source
gf	-254.80	kJ/mol	Joback Method
hf	-492.61	kJ/mol	Joback Method
hfus	41.83	kJ/mol	Joback Method
hvap	90.68	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	3.739		Crippen Method
mcvol	244.530	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	3572.00		NIST Webbook
rinpol	3572.00		NIST Webbook
tb	936.12	K	Joback Method
tc	1187.55	K	Joback Method
tf	634.11	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.30	J/mol×K	936.12	Joback Method
cpg	672.57	J/mol×K	1145.64	Joback Method
cpg	668.48	J/mol×K	1103.74	Joback Method
cpg	663.24	J/mol×K	1061.83	Joback Method
cpg	656.81	J/mol×K	1019.93	Joback Method
cpg	649.17	J/mol×K	978.02	Joback Method
cpg	675.54	J/mol×K	1187.55	Joback Method
dvisc	0.0000464	Pa×s	936.12	Joback Method

dvisc	0.0000564	Pa×s	885.79	Joback Method
dvisc	0.0000702	Pa×s	835.45	Joback Method
dvisc	0.0000898	Pa×s	785.12	Joback Method
dvisc	0.0001188	Pa×s	734.78	Joback Method
dvisc	0.0001638	Pa×s	684.45	Joback Method
dvisc	0.0002377	Pa×s	634.11	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=U381901&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