Diglycolic acid, 4-bromophenyl pentyl ester

Inchi: InChI=1S/C15H19BrO5/c1-2-3-4-9-20-14(17)10-19-11-15(18)21-13-7-5-12(16)6-8-13/h5-
InchiKey: BNEDGBJLGWUIJX-UHFFFAOYSA-N
Formula: C15H19BrO5
SMILES: CCCCCOC(=O)COCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 359.21

Physical Properties

Property code	Value	Unit	Source
gf	-380.32	kJ/mol	Joback Method
hf	-723.36	kJ/mol	Joback Method
hfus	40.30	kJ/mol	Joback Method
hvap	79.08	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.104		Crippen Method
mcvol	236.700	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	2895.00		NIST Webbook
rinpol	2895.00		NIST Webbook
tb	815.42	K	Joback Method
tc	1028.12	K	Joback Method
tf	524.10	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.65	J/mol×K	815.42	Joback Method
cpg	671.47	J/mol×K	850.87	Joback Method
cpg	683.26	J/mol×K	886.32	Joback Method
cpg	694.04	J/mol×K	921.77	Joback Method
cpg	703.80	J/mol×K	957.22	Joback Method
cpg	712.55	J/mol×K	992.67	Joback Method
cpg	720.30	J/mol×K	1028.12	Joback Method
dvisc	0.0004637	Pa×s	524.10	Joback Method

dvisc	0.0002925	Pa×s	572.65	Joback Method
dvisc	0.0001983	Pa×s	621.21	Joback Method
dvisc	0.0001422	Pa×s	669.76	Joback Method
dvisc	0.0001067	Pa×s	718.31	Joback Method
dvisc	0.0000830	Pa×s	766.87	Joback Method
dvisc	0.0000665	Pa×s	815.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381896&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