

Diglycolic acid, 4-bromophenyl butyl ester

Inchi:	InChI=1S/C14H17BrO5/c1-2-3-8-19-13(16)9-18-10-14(17)20-12-6-4-11(15)5-7-12/h4-7H
InchiKey:	XLRAIYDBMVXHII-UHFFFAOYSA-N
Formula:	C14H17BrO5
SMILES:	CCCCOC(=O)COCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	345.19

Physical Properties

Property code	Value	Unit	Source
gf	-388.74	kJ/mol	Joback Method
hf	-702.72	kJ/mol	Joback Method
hfus	37.71	kJ/mol	Joback Method
hvap	76.85	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.714		Crippen Method
mcvol	222.610	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	2763.00		NIST Webbook
rinpol	2763.00		NIST Webbook
tb	792.54	K	Joback Method
tc	1007.11	K	Joback Method
tf	512.83	K	Joback Method
vc	0.840	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.70	J/molxK	792.54	Joback Method
cpg	656.46	J/molxK	971.35	Joback Method
cpg	647.86	J/molxK	935.59	Joback Method
cpg	638.29	J/molxK	899.82	Joback Method
cpg	627.74	J/molxK	864.06	Joback Method
cpg	616.21	J/molxK	828.30	Joback Method
cpg	664.08	J/molxK	1007.11	Joback Method
dvisc	0.0000766	Paxs	792.54	Joback Method

dvisc	0.0000952	Paxs	745.92	Joback Method
dvisc	0.0001218	Paxs	699.30	Joback Method
dvisc	0.0001613	Paxs	652.68	Joback Method
dvisc	0.0002232	Paxs	606.07	Joback Method
dvisc	0.0003260	Paxs	559.45	Joback Method
dvisc	0.0005100	Paxs	512.83	Joback Method

Sources

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=U381895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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