

Diglycolic acid, 4-bromophenyl isobutyl ester

Inchi:	InChI=1S/C14H17BrO5/c1-10(2)7-19-13(16)8-18-9-14(17)20-12-5-3-11(15)4-6-12/h3-6,1
InchiKey:	FEEBAZSOAHUQMQ-UHFFFAOYSA-N
Formula:	C14H17BrO5
SMILES:	CC(C)COC(=O)COCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	345.19

Physical Properties

Property code	Value	Unit	Source
gf	-391.18	kJ/mol	Joback Method
hf	-708.00	kJ/mol	Joback Method
hfus	34.19	kJ/mol	Joback Method
hvap	76.47	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.570		Crippen Method
mcvol	222.610	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	2701.00		NIST Webbook
rinpol	2701.00		NIST Webbook
tb	792.10	K	Joback Method
tc	1009.85	K	Joback Method
tf	497.83	K	Joback Method
vc	0.834	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.29	J/molxK	792.10	Joback Method
cpg	616.98	J/molxK	828.39	Joback Method
cpg	628.65	J/molxK	864.68	Joback Method
cpg	639.30	J/molxK	900.98	Joback Method
cpg	648.93	J/molxK	937.27	Joback Method
cpg	657.55	J/molxK	973.56	Joback Method
cpg	665.15	J/molxK	1009.85	Joback Method
dvisc	0.0005657	Paxs	497.83	Joback Method

dvisc	0.0003421	Paxs	546.88	Joback Method
dvisc	0.0002247	Paxs	595.92	Joback Method
dvisc	0.0001574	Paxs	644.96	Joback Method
dvisc	0.0001159	Paxs	694.01	Joback Method
dvisc	0.0000889	Paxs	743.05	Joback Method
dvisc	0.0000704	Paxs	792.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U381894&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

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