4-Bromobutyric acid, 4-biphenyl ester

Inchi: InChI=1S/C16H15BrO2/c17-12-4-7-16(18)19-15-10-8-14(9-11-15)13-5-2-1-3-6-13/h1-3,5
InchiKey: SCOAEOMMVGBVGS-UHFFFAOYSA-N
Formula: C16H15BrO2
SMILES: O=C(CCCBr)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 319.19

Physical Properties

Property code	Value	Unit	Source
gf	79.43	kJ/mol	Joback Method
hf	-130.45	kJ/mol	Joback Method
hfus	32.96	kJ/mol	Joback Method
hvap	72.02	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.434		Crippen Method
mcvol	213.720	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	2502.00		NIST Webbook
tb	766.27	K	Joback Method
tc	1009.94	K	Joback Method
tf	467.40	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.25	J/mol×K	766.27	Joback Method
cpg	614.51	J/mol×K	969.33	Joback Method
cpg	604.74	J/mol×K	928.72	Joback Method
cpg	594.00	J/mol×K	888.11	Joback Method
cpg	582.22	J/mol×K	847.49	Joback Method
cpg	569.33	J/mol×K	806.88	Joback Method
cpg	623.37	J/mol×K	1009.94	Joback Method
dvisc	0.0001067	Pa×s	766.27	Joback Method
dvisc	0.0001337	Pa×s	716.46	Joback Method

dvisc	0.0001733	Pa×s	666.65	Joback Method
dvisc	0.0002342	Pa×s	616.84	Joback Method
dvisc	0.0003336	Pa×s	567.02	Joback Method
dvisc	0.0005089	Pa×s	517.21	Joback Method
dvisc	0.0008492	Pa×s	467.40	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=U354694&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