6-Bromohexanoic acid, 4-biphenyl ester

Inchi: InChI=1S/C18H19BrO2/c19-14-6-2-5-9-18(20)21-17-12-10-16(11-13-17)15-7-3-1-4-8-15/
InchiKey: DCBYCZLDASRQOO-UHFFFAOYSA-N
Formula: C18H19BrO2
SMILES: O=C(CCCCCBr)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 347.25

Physical Properties

Property code	Value	Unit	Source
gf	96.27	kJ/mol	Joback Method
hf	-171.73	kJ/mol	Joback Method
hfus	38.14	kJ/mol	Joback Method
hvap	76.47	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.214		Crippen Method
mcvol	241.900	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		NIST Webbook
tb	812.03	K	Joback Method
tc	1047.08	K	Joback Method
tf	489.94	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.50	J/mol×K	812.03	Joback Method
cpg	679.10	J/mol×K	851.21	Joback Method
cpg	692.53	J/mol×K	890.38	Joback Method
cpg	704.85	J/mol×K	929.56	Joback Method
cpg	716.15	J/mol×K	968.73	Joback Method
cpg	726.48	J/mol×K	1007.91	Joback Method
cpg	735.92	J/mol×K	1047.08	Joback Method
dvisc	0.0007136	Pa×s	489.94	Joback Method

dvisc	0.0004163	Pa×s	543.62	Joback Method
dvisc	0.0002675	Pa×s	597.30	Joback Method
dvisc	0.0001850	Pa×s	650.99	Joback Method
dvisc	0.0001353	Pa×s	704.67	Joback Method
dvisc	0.0001034	Pa×s	758.35	Joback Method
dvisc	0.0000819	Pa×s	812.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354722&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

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