6-Bromohexanoic acid, 2,3-dimethylphenyl ester

Inchi: InChI=1S/C14H19BrO2/c1-11-7-6-8-13(12(11)2)17-14(16)9-4-3-5-10-15/h6-8H,3-5,9-10H

InchiKey: LBVRMQLIVZFDEF-UHFFFAOYSA-N

Formula: C14H19BrO2

SMILES: Cc1cccc(OC(=O)CCCCCBr)c1C

Mol. weight [g/mol]: 299.20

Physical Properties

Property code	Value	Unit	Source
gf	-59.45	kJ/mol	Joback Method
hf	-337.17	kJ/mol	Joback Method
hfus	33.35	kJ/mol	Joback Method
hvap	65.95	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.164		Crippen Method
mcvol	209.300	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook
tb	698.81	K	Joback Method
tc	911.64	K	Joback Method
tf	430.96	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.68	J/mol×K	698.81	Joback Method
cpg	550.32	J/mol×K	734.28	Joback Method
cpg	564.07	J/mol×K	769.75	Joback Method
cpg	576.96	J/mol×K	805.23	Joback Method
cpg	589.02	J/mol×K	840.70	Joback Method
cpg	600.26	J/mol×K	876.17	Joback Method
cpg	610.73	J/mol×K	911.64	Joback Method
dvisc	0.0009647	Pa×s	430.96	Joback Method

dvisc	0.0005958	Pa×s	475.60	Joback Method
dvisc	0.0003997	Pa×s	520.24	Joback Method
dvisc	0.0002856	Pa×s	564.88	Joback Method
dvisc	0.0002144	Pa×s	609.53	Joback Method
dvisc	0.0001673	Pa×s	654.17	Joback Method
dvisc	0.0001348	Pa×s	698.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354719&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