6-Bromohexanoic acid, 3-ethylphenyl ester

Inchi: InChI=1S/C14H19BrO2/c1-2-12-7-6-8-13(11-12)17-14(16)9-4-3-5-10-15/h6-8,11H,2-5,9-
InchiKey: CGPARSXTTAMAJJ-UHFFFAOYSA-N
Formula: C14H19BrO2
SMILES: CCc1cccc(OC(=O)CCCCCBr)c1
Mol. weight [g/mol]: 299.20

Physical Properties

Property code	Value	Unit	Source
gf	-49.82	kJ/mol	Joback Method
hf	-325.70	kJ/mol	Joback Method
hfus	33.74	kJ/mol	Joback Method
hvap	65.29	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.110		Crippen Method
mcvol	209.300	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	2093.00		NIST Webbook
rinpol	2093.00		NIST Webbook
tb	693.83	K	Joback Method
tc	905.84	K	Joback Method
tf	418.44	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.57	J/mol×K	693.83	Joback Method
cpg	601.62	J/mol×K	870.50	Joback Method
cpg	590.31	J/mol×K	835.17	Joback Method
cpg	578.19	J/mol×K	799.83	Joback Method
cpg	565.21	J/mol×K	764.50	Joback Method
cpg	551.35	J/mol×K	729.16	Joback Method
cpg	612.15	J/mol×K	905.84	Joback Method
dvisc	0.0001352	Pa×s	693.83	Joback Method

dvisc	0.0001703	Pa×s	647.93	Joback Method
dvisc	0.0002223	Pa×s	602.03	Joback Method
dvisc	0.0003032	Pa×s	556.13	Joback Method
dvisc	0.0004373	Pa×s	510.24	Joback Method
dvisc	0.0006780	Pa×s	464.34	Joback Method
dvisc	0.0011575	Pa×s	418.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354718&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