6-Bromohexanoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C13H17BrO2/c1-11-6-5-7-12(10-11)16-13(15)8-3-2-4-9-14/h5-7,10H,2-4,8-9H2
InchiKey: YHTFVGXZYPGPKO-UHFFFAOYSA-N
Formula: C13H17BrO2
SMILES: Cc1cccc(OC(=O)CCCCCBr)c1
Mol. weight [g/mol]: 285.18

Physical Properties

Property code	Value	Unit	Source
gf	-58.24	kJ/mol	Joback Method
hf	-305.06	kJ/mol	Joback Method
hfus	31.15	kJ/mol	Joback Method
hvap	63.06	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.856		Crippen Method
mcvol	195.210	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	670.95	K	Joback Method
tc	886.24	K	Joback Method
tf	407.17	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.55	J/mol×K	670.95	Joback Method
cpg	498.85	J/mol×K	706.83	Joback Method
cpg	512.25	J/mol×K	742.71	Joback Method
cpg	524.79	J/mol×K	778.59	Joback Method
cpg	536.50	J/mol×K	814.48	Joback Method
cpg	547.42	J/mol×K	850.36	Joback Method
cpg	557.57	J/mol×K	886.24	Joback Method
dvisc	0.0012407	Pa×s	407.17	Joback Method

dvisc	0.0007382	Pa×s	451.13	Joback Method
dvisc	0.0004816	Pa×s	495.10	Joback Method
dvisc	0.0003369	Pa×s	539.06	Joback Method
dvisc	0.0002487	Pa×s	583.02	Joback Method
dvisc	0.0001916	Pa×s	626.99	Joback Method
dvisc	0.0001527	Pa×s	670.95	Joback Method

Sources

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=U307615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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