5-Bromovaleric acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C13H17BrO2/c1-10-7-11(2)9-12(8-10)16-13(15)5-3-4-6-14/h7-9H,3-6H2,1-2H3
InchiKey: AKENPROYQNLQBL-UHFFFAOYSA-N
Formula: C13H17BrO2
SMILES: Cc1cc(C)cc(OC(=O)CCCCBr)c1
Mol. weight [g/mol]: 285.18

Physical Properties

Property code	Value	Unit	Source
gf	-67.87	kJ/mol	Joback Method
hf	-316.53	kJ/mol	Joback Method
hfus	30.76	kJ/mol	Joback Method
hvap	63.72	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.774		Crippen Method
mcvol	195.210	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1887.00		NIST Webbook
tb	675.93	K	Joback Method
tc	892.07	K	Joback Method
tf	419.69	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.63	J/mol×K	675.93	Joback Method
cpg	545.97	J/mol×K	856.05	Joback Method
cpg	535.12	J/mol×K	820.02	Joback Method
cpg	523.48	J/mol×K	784.00	Joback Method
cpg	511.04	J/mol×K	747.98	Joback Method
cpg	497.76	J/mol×K	711.95	Joback Method
cpg	556.06	J/mol×K	892.07	Joback Method
dvisc	0.0001518	Pa×s	675.93	Joback Method
dvisc	0.0001876	Pa×s	633.22	Joback Method

dvisc	0.0002389	Pa×s	590.52	Joback Method
dvisc	0.0003160	Pa×s	547.81	Joback Method
dvisc	0.0004382	Pa×s	505.10	Joback Method
dvisc	0.0006456	Pa×s	462.40	Joback Method
dvisc	0.0010290	Pa×s	419.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307643&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