2-Bromobenzoic acid, 2-methylpentyl ester

Inchi: InChI=1S/C13H17BrO2/c1-3-6-10(2)9-16-13(15)11-7-4-5-8-12(11)14/h4-5,7-8,10H,3,6,9H
InchiKey: SYZFLJCRIOWUOH-UHFFFAOYSA-N
Formula: C13H17BrO2
SMILES: CCCC(C)COC(=O)c1ccccc1Br
Mol. weight [g/mol]: 285.18

Physical Properties

Property code	Value	Unit	Source
gf	-60.68	kJ/mol	Joback Method
hf	-310.34	kJ/mol	Joback Method
hfus	27.63	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.042		Crippen Method
mcvol	195.210	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	1832.00		NIST Webbook
rinpol	1832.00		NIST Webbook
tb	670.51	K	Joback Method
tc	889.92	K	Joback Method
tf	392.17	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.07	J/mol×K	670.51	Joback Method
cpg	549.02	J/mol×K	853.35	Joback Method
cpg	537.97	J/mol×K	816.78	Joback Method
cpg	526.09	J/mol×K	780.21	Joback Method
cpg	513.33	J/mol×K	743.65	Joback Method
cpg	499.67	J/mol×K	707.08	Joback Method
cpg	559.26	J/mol×K	889.92	Joback Method
dvisc	0.0001416	Pa×s	670.51	Joback Method

dvisc	0.0001809	Pa×s	624.12	Joback Method
dvisc	0.0002403	Pa×s	577.73	Joback Method
dvisc	0.0003354	Pa×s	531.34	Joback Method
dvisc	0.0004991	Pa×s	484.95	Joback Method
dvisc	0.0008078	Pa×s	438.56	Joback Method
dvisc	0.0014652	Pa×s	392.17	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=U354673&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