3-Bromobenzoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C15H13BrO2/c1-10-6-11(2)8-14(7-10)18-15(17)12-4-3-5-13(16)9-12/h3-9H,1-2

InchiKey: DBDKZGDUFHPWSD-UHFFFAOYSA-N

Formula: C15H13BrO2

SMILES: Cc1cc(C)cc(OC(=O)c2cccc(Br)c2)c1

Mol. weight [g/mol]: 305.17

Physical Properties

Property code	Value	Unit	Source
gf	51.75	kJ/mol	Joback Method
hf	-132.75	kJ/mol	Joback Method
hfus	29.59	kJ/mol	Joback Method
hvap	71.11	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.285		Crippen Method
mcvol	199.630	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
rinpol	2115.00		NIST Webbook
tb	753.35	K	Joback Method
tc	1003.66	K	Joback Method
tf	481.17	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.42	J/mol×K	753.35	Joback Method
cpg	512.89	J/mol×K	795.07	Joback Method
cpg	525.22	J/mol×K	836.79	Joback Method
cpg	536.49	J/mol×K	878.50	Joback Method
cpg	546.72	J/mol×K	920.22	Joback Method
cpg	555.98	J/mol×K	961.94	Joback Method
cpg	564.30	J/mol×K	1003.66	Joback Method
dvisc	0.0006823	Pa×s	481.17	Joback Method
dvisc	0.0004529	Pa×s	526.53	Joback Method

dvisc	0.0003208	Pa×s	571.90	Joback Method
dvisc	0.0002390	Pa×s	617.26	Joback Method
dvisc	0.0001854	Pa×s	662.62	Joback Method
dvisc	0.0001486	Pa×s	707.99	Joback Method
dvisc	0.0001223	Pa×s	753.35	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=U307550&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

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