2-Bromobenzoic acid, 3,5-difluorophenyl ester

Inchi: InChI=1S/C13H7BrF2O2/c14-12-4-2-1-3-11(12)13(17)18-10-6-8(15)5-9(16)7-10/h1-7H
InchiKey: VBHDOOCECZNZCX-UHFFFAOYSA-N
Formula: C13H7BrF2O2
SMILES: O=C(Oc1cc(F)cc(F)c1)c1ccccc1Br
Mol. weight [g/mol]: 313.09

Physical Properties

Property code	Value	Unit	Source
gf	-354.71	kJ/mol	Joback Method
hf	-483.69	kJ/mol	Joback Method
hfus	30.57	kJ/mol	Joback Method
hvap	65.03	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	3.947		Crippen Method
mcvol	174.990	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1799.00		NIST Webbook
tb	706.13	K	Joback Method
tc	944.68	K	Joback Method
tf	459.81	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.69	J/mol×K	706.13	Joback Method
cpg	423.80	J/mol×K	745.89	Joback Method
cpg	433.98	J/mol×K	785.65	Joback Method
cpg	443.28	J/mol×K	825.41	Joback Method
cpg	451.73	J/mol×K	865.16	Joback Method
cpg	459.37	J/mol×K	904.92	Joback Method
cpg	466.23	J/mol×K	944.68	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299014&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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