3-Trifluoromethylbenzoic acid, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C14H7BrF4O2/c15-11-7-10(16)4-5-12(11)21-13(20)8-2-1-3-9(6-8)14(17,18)19/

InchiKey: ORSKOPILQLSQCZ-UHFFFAOYSA-N

Formula: C14H7BrF4O2

SMILES: O=C(Oc1ccc(F)cc1Br)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 363.10

Physical Properties

Property code	Value	Unit	Source
gf	-733.07	kJ/mol	Joback Method
hf	-905.30	kJ/mol	Joback Method
hfus	31.91	kJ/mol	Joback Method
hvap	64.32	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	4.826		Crippen Method
mcvol	192.620	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	1763.00		NIST Webbook
rinpol	1763.00		NIST Webbook
tb	724.32	K	Joback Method
tc	950.72	K	Joback Method
tf	474.68	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.93	J/mol×K	724.32	Joback Method
cpg	492.73	J/mol×K	762.05	Joback Method
cpg	502.59	J/mol×K	799.79	Joback Method
cpg	511.57	J/mol×K	837.52	Joback Method
cpg	519.74	J/mol×K	875.25	Joback Method
cpg	527.16	J/mol×K	912.99	Joback Method
cpg	533.90	J/mol×K	950.72	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=U299041&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