Acetophenone, 3'-bromo, 2,2,2-trifluoro

Inchi: InChI=1S/C8H4BrF3O/c9-6-3-1-2-5(4-6)7(13)8(10,11)12/h1-4H
InchiKey: JOKNUXPHMQZTQB-UHFFFAOYSA-N
Formula: C8H4BrF3O
SMILES: O=C(c1cccc(Br)c1)C(F)(F)F
Mol. weight [g/mol]: 253.02

Physical Properties

Property code	Value	Unit	Source
gf	-576.93	kJ/mol	Joback Method
hf	-666.72	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	45.77	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.194		Crippen Method
mcvol	124.200	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	1090.00		NIST Webbook
tb	528.71	K	Joback Method
tc	746.73	K	Joback Method
tf	332.78	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.46	J/mol×K	528.71	Joback Method
cpg	264.08	J/mol×K	565.05	Joback Method
cpg	272.87	J/mol×K	601.38	Joback Method
cpg	280.89	J/mol×K	637.72	Joback Method
cpg	288.20	J/mol×K	674.05	Joback Method
cpg	294.86	J/mol×K	710.39	Joback Method
cpg	300.92	J/mol×K	746.73	Joback Method

Sources

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=R514971&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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