Bromo-4-fluoroacetophenone

Other names:	p-Fluorophenacyl bromide
	«omega»-Bromo-4-fluoroacetophenone
	4-Fluorophenacyl bromide
	Ethanone, 2-bromo-1-(4-fluorophenyl)-
	Acetophenone, 2-bromo-4'-fluoro-
	2-bromo-1-(4-fluorophenyl)ethan-1-one
Inchi:	InChI=1S/C8H6BrFO/c9-5-8(11)6-1-3-7(10)4-2-6/h1-4H,5H2
InchiKey:	ZJFWCELATJMDNO-UHFFFAOYSA-N
Formula:	C8H6BrFO
SMILES:	O=C(CBr)c1ccc(F)cc1
Mol. weight [g/mol]:	217.03
CAS:	403-29-2

Physical Properties

Property code	Value	Unit	Source
gf	-190.15	kJ/mol	Joback Method
hf	-265.75	kJ/mol	Joback Method
hfus	20.09	kJ/mol	Joback Method
hvap	48.70	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.403		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	533.40	K	Joback Method
tc	760.54	K	Joback Method
tf	329.18	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.95	J/mol×K	533.40	Joback Method
cpg	243.86	J/mol×K	571.26	Joback Method
cpg	253.06	J/mol×K	609.11	Joback Method

cpg	261.59	J/mol×K	646.97	Joback Method
cpg	269.49	J/mol×K	684.83	Joback Method
cpg	276.79	J/mol×K	722.68	Joback Method
cpg	283.53	J/mol×K	760.54	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=C403292&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume