Benzene, 1-(bromomethyl)-4-fluoro-

Other names:	Toluene, «alpha»-bromo-p-fluoro-
	p-Fluorobenzyl bromide
	4-Fluorobenzyl bromide
	«alpha»-Bromo-4-fluorotoluene
	«alpha»-bromo-p-fluorotoluene
Inchi:	InChI=1S/C7H6BrF/c8-5-6-1-3-7(9)4-2-6/h1-4H,5H2
InchiKey:	NVNPLEPBDPJYRZ-UHFFFAOYSA-N
Formula:	C7H6BrF
SMILES:	Fc1ccc(CBr)cc1
Mol. weight [g/mol]:	189.03
CAS:	459-46-1

Physical Properties

Property code	Value	Unit	Source
gf	-69.65	kJ/mol	Joback Method
hf	-132.53	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	39.73	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.721		Crippen Method
mcvol	105.000	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	456.65	K	Joback Method
tc	677.45	K	Joback Method
tf	267.98	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.66	J/mol×K	456.65	Joback Method
cpg	191.53	J/mol×K	493.45	Joback Method
cpg	200.73	J/mol×K	530.25	Joback Method
cpg	209.31	J/mol×K	567.05	Joback Method

cpg	217.30	J/mol×K	603.85	Joback Method
cpg	224.74	J/mol×K	640.65	Joback Method
cpg	231.65	J/mol×K	677.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.20	K	2.00	NIST Webbook

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=C459461&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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