2-FLUOROBENZYL BROMIDE

Other names:	o-Fluorobenzyl bromide
	Benzene, 1-(bromomethyl)-2-fluoro-
	«alpha»-bromo-o-fluorotoluene
Inchi:	InChI=1S/C7H6BrF/c8-5-6-3-1-2-4-7(6)9/h1-4H,5H2
InchiKey:	FFWQLZFIMNTUCZ-UHFFFAOYSA-N
Formula:	C7H6BrF
SMILES:	Fc1ccccc1CBr
Mol. weight [g/mol]:	189.03

Physical Properties

Property code	Value	Unit	Source
hf	-131.45	kJ/mol	Cheméo Relay (1.0)
hfus	15.90	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
log10ws	-2.51		Cheméo Relay (1.0)
logp	2.721		Crippen Method
mcvol	105.000	ml/mol	McGowan Method
tb	466.72	K	Cheméo Relay (1.0)
tc	675.65	K	Cheméo Relay (1.0)
tf	289.87	K	Cheméo Relay (1.0)

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C446480&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point