Benzene, 1-fluoro-3-(phenylmethyl)-

Inchi: InChI=1S/C13H11F/c14-13-8-4-7-12(10-13)9-11-5-2-1-3-6-11/h1-8,10H,9H2
InchiKey: QAJVVMNLYVCJCO-UHFFFAOYSA-N
Formula: C13H11F
SMILES: Fc1cccc(Cc2ccccc2)c1
Mol. weight [g/mol]: 186.22
CAS: 1496-00-0

Physical Properties

Property code	Value	Unit	Source
gf	78.96	kJ/mol	Joback Method
hf	-46.17	kJ/mol	Joback Method
hfus	20.20	kJ/mol	Joback Method
hvap	48.93	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.417		Crippen Method
mcvol	148.280	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
tb	554.45	K	Joback Method
tc	787.52	K	Joback Method
tf	302.22	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.72	J/mol×K	554.45	Joback Method
cpg	348.60	J/mol×K	593.30	Joback Method
cpg	363.31	J/mol×K	632.14	Joback Method
cpg	376.93	J/mol×K	670.99	Joback Method
cpg	389.52	J/mol×K	709.83	Joback Method
cpg	401.13	J/mol×K	748.68	Joback Method
cpg	411.84	J/mol×K	787.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1496000&Units=SI
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

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