Benzene, 1-(1,1-dimethylethyl)-4-(2-fluoroethyl)

Inchi: InChI=1S/C12H17F/c1-12(2,3)11-6-4-10(5-7-11)8-9-13/h4-7H,8-9H2,1-3H3
InchiKey: FCVVNGVMGCBLKR-UHFFFAOYSA-N
Formula: C12H17F
SMILES: CC(C)(C)c1ccc(CCF)cc1
Mol. weight [g/mol]: 180.26

Physical Properties

Property code	Value	Unit	Source
gf	-39.03	kJ/mol	Joback Method
hf	-270.81	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Joback Method
hvap	43.13	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.496		Crippen Method
mcvol	157.950	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1262.00		NIST Webbook
tb	501.66	K	Joback Method
tc	704.23	K	Joback Method
tf	266.95	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.25	J/mol×K	501.66	Joback Method
cpg	374.20	J/mol×K	535.42	Joback Method
cpg	390.13	J/mol×K	569.18	Joback Method
cpg	405.10	J/mol×K	602.95	Joback Method
cpg	419.15	J/mol×K	636.71	Joback Method
cpg	432.34	J/mol×K	670.47	Joback Method
cpg	444.70	J/mol×K	704.23	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=R515018&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