Benzene, 1-(2,2-dimethyl-1-methylenepropyl)-3-(trifluorome

Inchi: InChI=1S/C13H15F3/c1-9(12(2,3)4)10-6-5-7-11(8-10)13(14,15)16/h5-8H,1H2,2-4H3
InchiKey: HSVJYQINDWDIPW-UHFFFAOYSA-N
Formula: C13H15F3
SMILES: C=C(c1cccc(C(F)(F)F)c1)C(C)(C)C
Mol. weight [g/mol]: 228.25
CAS: 146558-45-4

Physical Properties

Property code	Value	Unit	Source
affp	831.10	kJ/mol	NIST Webbook
basg	802.20	kJ/mol	NIST Webbook
gf	-338.10	kJ/mol	Joback Method
hf	-576.78	kJ/mol	Joback Method
hfus	14.90	kJ/mol	Joback Method
hvap	41.84	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.765		Crippen Method
mcvol	171.280	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
tb	516.41	K	Joback Method
tc	715.98	K	Joback Method
tf	266.10	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.67	J/mol×K	516.41	Joback Method
cpg	421.55	J/mol×K	549.67	Joback Method
cpg	437.26	J/mol×K	582.93	Joback Method
cpg	451.86	J/mol×K	616.19	Joback Method
cpg	465.43	J/mol×K	649.46	Joback Method
cpg	478.04	J/mol×K	682.72	Joback Method
cpg	489.76	J/mol×K	715.98	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C146558454&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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