1,3,5-Tris(trifluoromethyl)benzene

Inchi: InChI=1S/C9H3F9/c10-7(11,12)4-1-5(8(13,14)15)3-6(2-4)9(16,17)18/h1-3H
InchiKey: ZMAUHKSOLPYPDB-UHFFFAOYSA-N
Formula: C9H3F9
SMILES: FC(F)(F)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 282.11
CAS: 729-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-1626.72	kJ/mol	Joback Method
hf	-1806.74	kJ/mol	Joback Method
hfus	17.81	kJ/mol	Joback Method
hvap	27.99	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.743		Crippen Method
mcvol	129.840	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
tb	391.50 ± 0.50	K	NIST Webbook
tc	583.33	K	Joback Method
tf	255.22	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.15	J/mol×K	425.70	Joback Method
cpg	309.69	J/mol×K	451.97	Joback Method
cpg	320.44	J/mol×K	478.24	Joback Method
cpg	330.45	J/mol×K	504.51	Joback Method
cpg	339.75	J/mol×K	530.78	Joback Method
cpg	348.37	J/mol×K	557.05	Joback Method
cpg	356.36	J/mol×K	583.33	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=C729817&Units=SI

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