Pyrogallol, tris(trifluoroacetate)

Inchi: InChI=1S/C12H3F9O6/c13-10(14,15)7(22)25-4-2-1-3-5(26-8(23)11(16,17)18)6(4)27-9(24
InchiKey: LVGFRJNVXPPMBM-UHFFFAOYSA-N
Formula: C12H3F9O6
SMILES: O=C(Oc1cccc(OC(=O)C(F)(F)F)c1OC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 414.13

Physical Properties

Property code	Value	Unit	Source
gf	-2303.22	kJ/mol	Joback Method
hf	-2603.06	kJ/mol	Joback Method
hfus	33.94	kJ/mol	Joback Method
hvap	62.13	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.090		Crippen Method
mcvol	194.430	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
tb	723.21	K	Joback Method
tc	904.30	K	Joback Method
tf	505.51	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.97	J/mol×K	723.21	Joback Method
cpg	561.18	J/mol×K	753.39	Joback Method
cpg	568.68	J/mol×K	783.57	Joback Method
cpg	575.51	J/mol×K	813.75	Joback Method
cpg	581.68	J/mol×K	843.93	Joback Method
cpg	587.24	J/mol×K	874.11	Joback Method
cpg	592.21	J/mol×K	904.30	Joback Method

Sources

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=U375769&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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