Orcinol, bis(pentafluoropropionate)

Other names: Resorcinol, 5-methyl, bis-PFP
Inchi: InChI=1S/C13H6F10O4/c1-5-2-6(26-8(24)10(14,15)12(18,19)20)4-7(3-5)27-9(25)11(16,1
InchiKey: LZPRQOUEDNESEP-UHFFFAOYSA-N
Formula: C13H6F10O4
SMILES: Cc1cc(OC(=O)C(F)(F)C(F)(F)F)cc(OC(=O)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 416.17

Physical Properties

Property code	Value	Unit	Source
gf	-2252.85	kJ/mol	Joback Method
hf	-2583.76	kJ/mol	Joback Method
hfus	29.41	kJ/mol	Joback Method
hvap	53.09	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.201		Crippen Method
mcvol	202.850	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	1116.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1143.00		NIST Webbook
tb	665.84	K	Joback Method
tc	839.39	K	Joback Method
tf	447.63	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.94	J/mol×K	665.84	Joback Method
cpg	589.07	J/mol×K	694.76	Joback Method
cpg	598.40	J/mol×K	723.69	Joback Method
cpg	606.99	J/mol×K	752.61	Joback Method
cpg	614.88	J/mol×K	781.54	Joback Method
cpg	622.12	J/mol×K	810.46	Joback Method

cpg	628.77	J/mol×K	839.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375930&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume