Pyrocatechol, TFA-PFP

Inchi: InChI=1S/C11H4F8O4/c12-9(13,11(17,18)19)7(20)22-5-3-1-2-4-6(5)23-8(21)10(14,15)16
InchiKey: TVYMIPKKIIWINS-UHFFFAOYSA-N
Formula: C11H4F8O4
SMILES: O=C(Oc1ccccc1OC(=O)C(F)(F)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 352.13

Physical Properties

Property code	Value	Unit	Source
gf	-1873.28	kJ/mol	Joback Method
hf	-2130.04	kJ/mol	Joback Method
hfus	25.87	kJ/mol	Joback Method
hvap	50.91	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.257		Crippen Method
mcvol	171.130	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	1022.00		NIST Webbook
rinpol	1022.00		NIST Webbook
tb	619.79	K	Joback Method
tc	798.95	K	Joback Method
tf	408.97	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.50	J/mol×K	619.79	Joback Method
cpg	472.36	J/mol×K	649.65	Joback Method
cpg	481.46	J/mol×K	679.51	Joback Method
cpg	489.82	J/mol×K	709.37	Joback Method
cpg	497.49	J/mol×K	739.23	Joback Method
cpg	504.51	J/mol×K	769.09	Joback Method
cpg	510.92	J/mol×K	798.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R335614&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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