

Pyrocatechol, TFA-HFB

Inchi:	InChI=1S/C12H4F10O4/c13-9(14,11(18,19)12(20,21)22)7(23)25-5-3-1-2-4-6(5)26-8(24)1
InchiKey:	OPQXYVMJHCSWCU-UHFFFAOYSA-N
Formula:	C12H4F10O4
SMILES:	O=C(Oc1ccccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	402.14

Physical Properties

Property code	Value	Unit	Source
gf	-2251.64	kJ/mol	Joback Method
hf	-2551.65	kJ/mol	Joback Method
hfus	27.21	kJ/mol	Joback Method
hvap	50.20	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.893		Crippen Method
mcvol	188.760	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1065.00		NIST Webbook
rinpol	1065.00		NIST Webbook
tb	637.98	K	Joback Method
tc	811.02	K	Joback Method
tf	423.84	K	Joback Method
vc	0.783	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.58	J/mol×K	637.98	Joback Method
cpg	540.46	J/mol×K	666.82	Joback Method
cpg	549.53	J/mol×K	695.66	Joback Method
cpg	557.83	J/mol×K	724.50	Joback Method
cpg	565.43	J/mol×K	753.34	Joback Method
cpg	572.36	J/mol×K	782.18	Joback Method
cpg	578.68	J/mol×K	811.02	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=R335609&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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