Hydroquinone, 2-trifluoroacetyl, bis-TFA

Inchi: InChI=1S/C12H3F9O5/c13-10(14,15)7(22)5-3-4(25-8(23)11(16,17)18)1-2-6(5)26-9(24)12
InchiKey: AQMJOBXEVCXZSQ-UHFFFAOYSA-N
Formula: C12H3F9O5
SMILES: O=C(Oc1ccc(OC(=O)C(F)(F)F)c(C(=O)C(F)(F)F)c1)C(F)(F)F
Mol. weight [g/mol]: 398.13

Physical Properties

Property code	Value	Unit	Source
gf	-2198.22	kJ/mol	Joback Method
hf	-2470.84	kJ/mol	Joback Method
hfus	32.75	kJ/mol	Joback Method
hvap	59.72	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.367		Crippen Method
mcvol	188.560	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	1152.00		NIST Webbook
rinpol	1152.00		NIST Webbook
tb	700.79	K	Joback Method
tc	881.41	K	Joback Method
tf	483.28	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.53	J/mol×K	700.79	Joback Method
cpg	537.92	J/mol×K	730.89	Joback Method
cpg	545.60	J/mol×K	761.00	Joback Method
cpg	552.61	J/mol×K	791.10	Joback Method
cpg	558.98	J/mol×K	821.20	Joback Method
cpg	564.76	J/mol×K	851.31	Joback Method
cpg	569.99	J/mol×K	881.41	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=R335421&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume