Hydroquinone, 2-trifluoroacetyl, bis-PFP

Inchi: InChI=1S/C14H3F13O5/c15-10(16,13(22,23)24)8(29)31-4-1-2-6(5(3-4)7(28)12(19,20)21)
InchiKey: VSBOBVMCUQMIIU-UHFFFAOYSA-N
Formula: C14H3F13O5
SMILES: O=C(c1cc(OC(=O)C(F)(F)C(F)(F)F)ccc1OC(=O)C(F)(F)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 498.15

Physical Properties

Property code	Value	Unit	Source
gf	-2954.94	kJ/mol	Joback Method
hf	-3314.06	kJ/mol	Joback Method
hfus	35.42	kJ/mol	Joback Method
hvap	58.31	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.638		Crippen Method
mcvol	223.820	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	1195.00		NIST Webbook
tb	737.17	K	Joback Method
tc	911.46	K	Joback Method
tf	513.02	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.13	J/mol×K	737.17	Joback Method
cpg	676.35	J/mol×K	766.22	Joback Method
cpg	683.81	J/mol×K	795.27	Joback Method
cpg	690.58	J/mol×K	824.32	Joback Method
cpg	696.71	J/mol×K	853.36	Joback Method
cpg	702.28	J/mol×K	882.41	Joback Method
cpg	707.34	J/mol×K	911.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R335416&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

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