Hydroquinone, bis(heptafluorobutyrate)

Other names: Hydroquinone, bis-HFB
Inchi: InChI=1S/C14H4F14O4/c15-9(16,11(19,20)13(23,24)25)7(29)31-5-1-2-6(4-3-5)32-8(30)1
InchiKey: QEHZFJKTGOGEHM-UHFFFAOYSA-N
Formula: C14H4F14O4
SMILES: O=C(Oc1ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 502.16

Physical Properties

Property code	Value	Unit	Source
gf	-3008.36	kJ/mol	Joback Method
hf	-3394.87	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	48.79	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.163		Crippen Method
mcvol	224.020	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinpol	1168.00		NIST Webbook
rinpol	1168.00		NIST Webbook
tb	674.36	K	Joback Method
tc	839.41	K	Joback Method
tf	453.58	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.83	J/mol×K	674.36	Joback Method
cpg	678.57	J/mol×K	701.87	Joback Method
cpg	687.44	J/mol×K	729.38	Joback Method
cpg	695.51	J/mol×K	756.89	Joback Method
cpg	702.86	J/mol×K	784.39	Joback Method
cpg	709.55	J/mol×K	811.90	Joback Method
cpg	715.64	J/mol×K	839.41	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=U364787&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