

Hydroquinone, 2-trifluoroacetyl, TFA-PFP

Inchi: InChI=1S/C13H3F11O5/c14-10(15,13(22,23)24)8(26)29-6-2-1-4(28-9(27)12(19,20)21)3-5
InchiKey: NIRJNJAMZLJKKS-UHFFFAOYSA-N
Formula: C13H3F11O5
SMILES: O=C(Oc1ccc(OC(=O)C(F)(F)C(F)(F)F)c(C(=O)C(F)(F)F)c1)C(F)(F)F
Mol. weight [g/mol]: 448.14

Physical Properties

Property code	Value	Unit	Source
gf	-2576.58	kJ/mol	Joback Method
hf	-2892.45	kJ/mol	Joback Method
hfus	34.09	kJ/mol	Joback Method
hvap	59.02	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.002		Crippen Method
mcvol	206.190	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
tb	718.98	K	Joback Method
tc	895.63	K	Joback Method
tf	498.15	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.63	J/molxK	718.98	Joback Method
cpg	606.94	J/molxK	748.42	Joback Method
cpg	614.52	J/molxK	777.86	Joback Method
cpg	621.41	J/molxK	807.31	Joback Method
cpg	627.66	J/molxK	836.75	Joback Method
cpg	633.33	J/molxK	866.19	Joback Method
cpg	638.46	J/molxK	895.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R335436&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvac:	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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