Benzhydrol, 4-trifluoromethyl-

Inchi: InChI=1S/C14H11F3O/c15-14(16,17)12-8-6-11(7-9-12)13(18)10-4-2-1-3-5-10/h1-9,13,18
InchiKey: LIZDGCXCDJOWBS-UHFFFAOYSA-N
Formula: C14H11F3O
SMILES: OC(c1ccccc1)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 252.23
CAS: 395-23-3

Physical Properties

Property code	Value	Unit	Source
gf	-438.66	kJ/mol	Joback Method
hf	-625.29	kJ/mol	Joback Method
hfus	22.10	kJ/mol	Joback Method
hvap	64.52	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.787		Crippen Method
mcvol	171.780	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
tb	664.38	K	Joback Method
tc	872.53	K	Joback Method
tf	362.91	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.41	J/mol×K	664.38	Joback Method
cpg	467.92	J/mol×K	699.07	Joback Method
cpg	479.47	J/mol×K	733.76	Joback Method
cpg	490.12	J/mol×K	768.46	Joback Method
cpg	499.94	J/mol×K	803.15	Joback Method
cpg	509.00	J/mol×K	837.84	Joback Method
cpg	517.38	J/mol×K	872.53	Joback Method

Sources

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=C395233&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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