Hexafluoro-2-(p-tolyl)-i-propanol

Other names: Hexafluoro-2-(p-tolyl)-i-propanol
Inchi: InChI=1S/C10H8F6O/c1-6-2-4-7(5-3-6)8(17,9(11,12)13)10(14,15)16/h2-5,17H,1H3
InchiKey: AOAVZPXKNQAALI-UHFFFAOYSA-N
Formula: C10H8F6O
SMILES: Cc1ccc(C(O)(C(F)(F)F)C(F)(F)F)cc1
Mol. weight [g/mol]: 258.16

Physical Properties

Property code	Value	Unit	Source
af	0.5551		Cheméo Relay (1.0)
gf	-1161.06	kJ/mol	Joback Method
hf	-1356.69	kJ/mol	Cheméo Relay (1.0)
hfus	15.63	kJ/mol	Joback Method
hvap	73.93	kJ/mol	Cheméo Relay (1.0)
ie	9.30	eV	Cheméo Relay (1.0)
log10ws	-3.22		Cheméo Relay (1.0)
logp	3.307		Crippen Method
mcvol	144.490	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
tb	455.00	K	NIST Webbook
tc	657.27	K	Cheméo Relay (1.0)
tf	252.06	K	Cheméo Relay (1.0)
vc	0.525	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.29	J/mol×K	537.97	Joback Method
cpg	382.49	J/mol×K	566.88	Joback Method
cpg	392.84	J/mol×K	595.79	Joback Method
cpg	402.40	J/mol×K	624.70	Joback Method
cpg	411.23	J/mol×K	653.60	Joback Method
cpg	419.38	J/mol×K	682.51	Joback Method
cpg	426.90	J/mol×K	711.42	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2010619&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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