

p-(Heptafluoroisopropyl)toluene

Inchi:	InChI=1S/C10H7F7/c1-6-2-4-7(5-3-6)8(11,9(12,13)14)10(15,16)17/h2-5H,1H3
InchiKey:	XEFRSBQTXVJYKZ-UHFFFAOYSA-N
Formula:	C10H7F7
SMILES:	Cc1ccc(C(F)(C(F)(F)F)C(F)(F)F)cc1
Mol. weight [g/mol]:	260.15

Physical Properties

Property code	Value	Unit	Source
af	0.4041		Cheméo Relay (1.0)
gf	-1219.05	kJ/mol	Joback Method
hf	-1449.37	kJ/mol	Cheméo Relay (1.0)
hfus	14.63	kJ/mol	Joback Method
hvap	44.45	kJ/mol	Cheméo Relay (1.0)
ie	9.42	eV	Cheméo Relay (1.0)
log10ws	-4.34		Cheméo Relay (1.0)
logp	4.284		Crippen Method
mcvol	140.390	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
tb	405.08	K	Cheméo Relay (1.0)
tc	576.52	K	Cheméo Relay (1.0)
tf	202.20	K	Cheméo Relay (1.0)
vc	0.516	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.31	J/mol×K	445.06	Joback Method
cpg	336.11	J/mol×K	473.73	Joback Method
cpg	348.93	J/mol×K	502.41	Joback Method
cpg	360.82	J/mol×K	531.08	Joback Method
cpg	371.83	J/mol×K	559.76	Joback Method
cpg	382.01	J/mol×K	588.43	Joback Method
cpg	391.41	J/mol×K	617.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2396261&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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

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