

4-Methylphenol, heptafluorobutyrate

Other names:	p-Cresol, heptafluorobutanoate
Inchi:	InChI=1S/C11H7F7O2/c1-6-2-4-7(5-3-6)20-8(19)9(12,13)10(14,15)11(16,17)18/h2-5H,1H
InchiKey:	VCCSPRCTQRXVBV-UHFFFAOYSA-N
Formula:	C11H7F7O2
SMILES:	Cc1ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]:	304.16

Physical Properties

Property code	Value	Unit	Source
gf	-1444.55	kJ/mol	Joback Method
hf	-1689.13	kJ/mol	Joback Method
hfus	20.00	kJ/mol	Joback Method
hvap	42.57	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.733		Crippen Method
mcvol	161.920	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1042.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
tb	544.23	K	Joback Method
tc	723.63	K	Joback Method
tf	336.22	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.92	J/molxK	544.23	Joback Method
cpg	426.16	J/molxK	574.13	Joback Method
cpg	437.49	J/molxK	604.03	Joback Method
cpg	447.97	J/molxK	633.93	Joback Method
cpg	457.66	J/molxK	663.83	Joback Method

cpg	466.59	J/mol×K	693.73	Joback Method
cpg	474.82	J/mol×K	723.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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