Heptafluorobutyric acid, 4-methoxyphenyl ester

Other names: Heptafluorobutyric acid, 4-methoxyphenyl ester
Inchi: InChI=1S/C11H7F7O3/c1-20-6-2-4-7(5-3-6)21-8(19)9(12,13)10(14,15)11(16,17)18/h2-5H
InchiKey: MAXXAEQHDYJTRK-UHFFFAOYSA-N
Formula: C11H7F7O3
SMILES: COc1ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 320.16

Physical Properties

Property code	Value	Unit	Source
hf	-1890.06	kJ/mol	Cheméo Relay (1.0)
hfus	21.19	kJ/mol	Joback Method
hvap	67.87	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
log10ws	-4.78		Cheméo Relay (1.0)
logp	3.434		Crippen Method
mcvol	167.790	ml/mol	McGowan Method
rinpol	1177.00		NIST Webbook
tb	485.52	K	Cheméo Relay (1.0)
tf	274.12	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.54	J/mol×K	566.65	Joback Method
cpg	450.35	J/mol×K	596.42	Joback Method
cpg	461.33	J/mol×K	626.18	Joback Method
cpg	471.52	J/mol×K	655.95	Joback Method
cpg	480.95	J/mol×K	685.71	Joback Method
cpg	489.68	J/mol×K	715.48	Joback Method
cpg	497.74	J/mol×K	745.25	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80527453&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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