methyl 3,5-diCF3-benzoate radical

Inchi:	InChI=1S/C10H6F6O2/c1-18-8(17)5-2-6(9(11,12)13)4-7(3-5)10(14,15)16/h2-4H,1H3
InchiKey:	LTYNBDAJUXZFHP-UHFFFAOYSA-N
Formula:	C10H6F6O2
SMILES:	COC(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	272.14
CAS:	26107-80-2

Physical Properties

Property code	Value	Unit	Source
ea	1.01 ± 0.09	eV	NIST Webbook
ea	0.98 ± 0.09	eV	NIST Webbook
gf	-1270.63	kJ/mol	Joback Method
hf	-1475.10	kJ/mol	Joback Method
hfus	21.36	kJ/mol	Joback Method
hvap	43.12	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.511		Crippen Method
mcvol	146.060	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
tb	530.29	K	Joback Method
tc	710.85	K	Joback Method
tf	334.46	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.62	J/mol×K	530.29	Joback Method
cpg	367.67	J/mol×K	560.38	Joback Method
cpg	378.00	J/mol×K	590.48	Joback Method
cpg	387.64	J/mol×K	620.57	Joback Method
cpg	396.62	J/mol×K	650.66	Joback Method
cpg	404.98	J/mol×K	680.75	Joback Method
cpg	412.74	J/mol×K	710.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26107802&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ea:	Electron affinity
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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