4-Methylbenzoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C13H10F8O2/c1-7-2-4-8(5-3-7)9(22)23-6-11(16,17)13(20,21)12(18,19)10(14)1

InchiKey: VFQPUOOYILXUNL-UHFFFAOYSA-N

Formula: C13H10F8O2

SMILES: Cc1ccc(C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)cc1

Mol. weight [g/mol]: 350.20

Physical Properties

Property code	Value	Unit	Source
gf	-1624.96	kJ/mol	Joback Method
hf	-1931.80	kJ/mol	Joback Method
hfus	24.74	kJ/mol	Joback Method
hvap	45.81	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.323		Crippen Method
mcvol	191.870	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
tb	588.82	K	Joback Method
tc	761.20	K	Joback Method
tf	344.35	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.10	J/mol×K	588.82	Joback Method
cpg	531.03	J/mol×K	617.55	Joback Method
cpg	543.06	J/mol×K	646.28	Joback Method
cpg	554.26	J/mol×K	675.01	Joback Method
cpg	564.66	J/mol×K	703.74	Joback Method
cpg	574.33	J/mol×K	732.47	Joback Method
cpg	583.30	J/mol×K	761.20	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume