4-Methoxyphenol, heptafluorobutyrate

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
CAS: 80527-45-3

Physical Properties

Property code	Value	Unit	Source
gf	-1549.55	kJ/mol	Joback Method
hf	-1821.35	kJ/mol	Joback Method
hfus	21.19	kJ/mol	Joback Method
hvap	44.98	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.434		Crippen Method
mcvol	167.790	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	1177.00		NIST Webbook
tb	566.65	K	Joback Method
tc	745.25	K	Joback Method
tf	358.45	K	Joback Method
vc	0.678	m3/kmol	Joback Method

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:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C80527453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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