Heptyl 2,3,4,5,6-pentafluorobenzoate

Other names: heptyl pentafluorobenzoate
1-Heptanol, pentafluorobenzoate
Inchi: InChI=1S/C14H15F5O2/c1-2-3-4-5-6-7-21-14(20)8-9(15)11(17)13(19)12(18)10(8)16/h2-7
InchiKey: OXDIHQFKUKTZOU-UHFFFAOYSA-N
Formula: C14H15F5O2
SMILES: CCCCCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 310.26

Physical Properties

Property code	Value	Unit	Source
gf	-1076.71	kJ/mol	Joback Method
hf	-1378.46	kJ/mol	Joback Method
hfus	42.30	kJ/mol	Joback Method
hvap	57.41	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.509		Crippen Method
mcvol	200.650	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	1538.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1519.00		NIST Webbook
ripol	1802.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1778.00		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1814.00		NIST Webbook
ripol	1812.00		NIST Webbook

ripol	1788.00		NIST Webbook
ripol	1788.00		NIST Webbook
tb	643.94	K	Joback Method
tc	813.51	K	Joback Method
tf	411.67	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.24	J/mol×K	643.94	Joback Method
cpg	544.78	J/mol×K	672.20	Joback Method
cpg	556.78	J/mol×K	700.46	Joback Method
cpg	568.22	J/mol×K	728.73	Joback Method
cpg	579.12	J/mol×K	756.99	Joback Method
cpg	589.47	J/mol×K	785.25	Joback Method
cpg	599.29	J/mol×K	813.51	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373586&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume