2-Methylpropenoic acid, pentafluorophenyl ester

Other names: 2,3,4,5,6-Pentafluorophenyl 2-methylacrylate
2-Propenoic acid, 2-methyl-, pentafluorophenyl ester
Pentafluorophenyl methacrylate
2-propenyl pentaflurobenzoate

Inchi: InChI=1S/C10H5F5O2/c1-3(2)10(16)17-9-7(14)5(12)4(11)6(13)8(9)15/h1H2,2H3

InchiKey: NIJWSVFNELSKMF-UHFFFAOYSA-N

Formula: C10H5F5O2

SMILES: C=C(C)C(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 252.14

CAS: 13642-97-2

Physical Properties

Property code	Value	Unit	Source
gf	-1031.10	kJ/mol	Joback Method
hf	-1180.26	kJ/mol	Joback Method
hfus	29.35	kJ/mol	Joback Method
hvap	47.92	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.864		Crippen Method
mcvol	139.990	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	1104.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1111.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1463.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1470.00		NIST Webbook
tb	548.98	K	Joback Method
tc	727.46	K	Joback Method
tf	350.87	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.63	J/mol×K	548.98	Joback Method
cpg	329.53	J/mol×K	578.73	Joback Method
cpg	338.06	J/mol×K	608.47	Joback Method
cpg	346.22	J/mol×K	638.22	Joback Method
cpg	354.02	J/mol×K	667.97	Joback Method
cpg	361.45	J/mol×K	697.71	Joback Method
cpg	368.50	J/mol×K	727.46	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13642972&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