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

Other names: Pentafluorobenzoic acid, 3-methylbutyl ester
3-methylbutyl pentafluorobenzoate
Inchi: InChI=1S/C12H11F5O2/c1-5(2)3-4-19-12(18)6-7(13)9(15)11(17)10(16)8(6)14/h5H,3-4H2
InchiKey: GMWUXUNXUBNVOC-UHFFFAOYSA-N
Formula: C12H11F5O2
SMILES: CC(C)CCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 282.21
CAS: 99483-16-6

Physical Properties

Property code	Value	Unit	Source
gf	-1095.99	kJ/mol	Joback Method
hf	-1342.46	kJ/mol	Joback Method
hfus	33.60	kJ/mol	Joback Method
hvap	52.58	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.585		Crippen Method
mcvol	172.470	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1308.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1286.00		NIST Webbook
ripol	1541.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1558.00		NIST Webbook
tb	597.74	K	Joback Method
tc	771.09	K	Joback Method
tf	374.13	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.19	J/mol×K	597.74	Joback Method
cpg	444.56	J/mol×K	626.63	Joback Method
cpg	455.45	J/mol×K	655.52	Joback Method
cpg	465.86	J/mol×K	684.41	Joback Method
cpg	475.78	J/mol×K	713.31	Joback Method
cpg	485.23	J/mol×K	742.20	Joback Method
cpg	494.19	J/mol×K	771.09	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99483166&Units=SI

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