3-Methylbutan-2-yl 2,3,4,5,6-pentafluorobenzoate

Other names: 1,2-dimethylpropyl pentafluorobenzoate

Pentafluorobenzoic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C12H11F5O2/c1-4(2)5(3)19-12(18)6-7(13)9(15)11(17)10(16)8(6)14/h4-5H,1-3

InchiKey: WYIQGISADCVNPE-UHFFFAOYSA-N

Formula: C12H11F5O2

SMILES: CC(C)C(C)OC(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 282.21

CAS: 99483-14-4

Physical Properties

Property code	Value	Unit	Source
gf	-1098.43	kJ/mol	Joback Method
hf	-1347.74	kJ/mol	Joback Method
hfus	30.07	kJ/mol	Joback Method
hvap	52.19	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.583		Crippen Method
mcvol	172.470	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	1264.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1246.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1490.00		NIST Webbook
tb	597.30	K	Joback Method
tc	773.55	K	Joback Method
tf	359.13	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.62	J/mol×K	597.30	Joback Method
cpg	445.22	J/mol×K	626.67	Joback Method
cpg	456.33	J/mol×K	656.05	Joback Method
cpg	466.92	J/mol×K	685.42	Joback Method
cpg	477.02	J/mol×K	714.80	Joback Method
cpg	486.60	J/mol×K	744.17	Joback Method
cpg	495.68	J/mol×K	773.55	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=C99483144&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume