Pentafluorobenzoic acid, 3-methylbutyl ester

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

Physical Properties

Property code	Value	Unit	Source
hf	-1158.39	kJ/mol	Cheméo Relay (1.0)
hfus	33.60	kJ/mol	Joback Method
hvap	66.86	kJ/mol	Cheméo Relay (1.0)
ie	9.76	eV	Cheméo Relay (1.0)
log10ws	-5.86		Cheméo Relay (1.0)
logp	3.585		Crippen Method
mcvol	172.470	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1283.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1541.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1559.00		NIST Webbook
tb	501.17	K	Cheméo Relay (1.0)
tc	686.26	K	Cheméo Relay (1.0)
tf	252.29	K	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99483166&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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