3-Methylbut-3-enyl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C12H9F5O2/c1-5(2)3-4-19-12(18)6-7(13)9(15)11(17)10(16)8(6)14/h1,3-4H2,2H

InchiKey: BTSWFQQPZGDXBF-UHFFFAOYSA-N

Formula: C12H9F5O2

SMILES: C=C(C)CCOC(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 280.19

Physical Properties

Property code	Value	Unit	Source
gf	-1014.26	kJ/mol	Joback Method
hf	-1221.54	kJ/mol	Joback Method
hfus	34.53	kJ/mol	Joback Method
hvap	52.37	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.505		Crippen Method
mcvol	168.170	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1322.00		NIST Webbook
rinpol	1322.00		NIST Webbook
tb	594.74	K	Joback Method
tc	770.31	K	Joback Method
tf	373.41	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.87	J/mol×K	594.74	Joback Method
cpg	422.53	J/mol×K	624.00	Joback Method
cpg	432.72	J/mol×K	653.26	Joback Method
cpg	442.45	J/mol×K	682.53	Joback Method
cpg	451.71	J/mol×K	711.79	Joback Method
cpg	460.52	J/mol×K	741.05	Joback Method
cpg	468.87	J/mol×K	770.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373582&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume