3-Methylbut-2-en-1-yl 2,3,4,5,6-pentafluorobenzoate

Other names: Pentafluorobenzoic acid, 3-methylbut-2-enyl ester
Inchi: InChI=1S/C12H9F5O2/c1-5(2)3-4-19-12(18)6-7(13)9(15)11(17)10(16)8(6)14/h3H,4H2,1-
InchiKey: DCHOROKVNQCKKX-UHFFFAOYSA-N
Formula: C12H9F5O2
SMILES: CC(C)=CCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 280.19
CAS: 958998-46-4

Physical Properties

Property code	Value	Unit	Source
gf	-1021.88	kJ/mol	Joback Method
hf	-1229.75	kJ/mol	Joback Method
hfus	36.01	kJ/mol	Joback Method
hvap	53.00	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.505		Crippen Method
mcvol	168.170	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	1337.00		NIST Webbook
rinpol	1337.00		NIST Webbook
tb	602.22	K	Joback Method
tc	781.38	K	Joback Method
tf	370.09	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.02	J/mol×K	602.22	Joback Method
cpg	422.74	J/mol×K	632.08	Joback Method
cpg	432.97	J/mol×K	661.94	Joback Method
cpg	442.72	J/mol×K	691.80	Joback Method
cpg	451.98	J/mol×K	721.66	Joback Method
cpg	460.78	J/mol×K	751.52	Joback Method

cpg	469.11	J/mol×K	781.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C958998464&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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