

1-methyl-3-butenyl pentafluorobenzoate

Inchi: InChI=1S/C12H9F5O2/c1-3-4-5(2)19-12(18)6-7(13)9(15)11(17)10(16)8(6)14/h3,5H,1,4H
InchiKey: WPDVFLKYMQQYGM-UHFFFAOYSA-N
Formula: C12H9F5O2
SMILES: C=CCC(C)OC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 280.19

Physical Properties

Property code	Value	Unit	Source
gf	-1008.15	kJ/mol	Joback Method
hf	-1217.03	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	51.91	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.503		Crippen Method
mcvol	168.170	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1241.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1242.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1541.00		NIST Webbook
ripol	1540.00		NIST Webbook
tb	594.42	K	Joback Method
tc	770.45	K	Joback Method
tf	372.37	K	Joback Method
vc	0.689	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.53	J/mol×K	594.42	Joback Method
cpg	423.29	J/mol×K	623.76	Joback Method
cpg	433.57	J/mol×K	653.10	Joback Method
cpg	443.37	J/mol×K	682.44	Joback Method
cpg	452.70	J/mol×K	711.77	Joback Method
cpg	461.56	J/mol×K	741.11	Joback Method
cpg	469.95	J/mol×K	770.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R311841&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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