(E)-2-butenyl pentaflurobenzoate

Inchi: InChI=1S/C11H7F5O2/c1-2-3-4-18-11(17)5-6(12)8(14)10(16)9(15)7(5)13/h2-3H,4H2,1H3
InchiKey: RJSCWKIHRDEMHX-NSCUHMNNSA-N
Formula: C11H7F5O2
SMILES: CC=CCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 266.16

Physical Properties

Property code	Value	Unit	Source
gf	-1021.75	kJ/mol	Joback Method
hf	-1199.32	kJ/mol	Joback Method
hfus	34.73	kJ/mol	Joback Method
hvap	50.69	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.115		Crippen Method
mcvol	154.080	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	1228.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1228.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
tb	579.46	K	Joback Method
tc	757.46	K	Joback Method
tf	372.78	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.48	J/mol×K	579.46	Joback Method
cpg	375.26	J/mol×K	609.13	Joback Method
cpg	384.61	J/mol×K	638.79	Joback Method
cpg	393.53	J/mol×K	668.46	Joback Method
cpg	402.02	J/mol×K	698.13	Joback Method
cpg	410.10	J/mol×K	727.79	Joback Method
cpg	417.75	J/mol×K	757.46	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=R311896&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