Pentafluorobenzoic acid, undec-2-enyl ester

Inchi: InChI=1S/C18H21F5O2/c1-2-3-4-5-6-7-8-9-10-11-25-18(24)12-13(19)15(21)17(23)16(22
InchiKey: MFMYOCNWFRJXBK-MDZDMXLPSA-N
Formula: C18H21F5O2
SMILES: CCCCCCCCC=CCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 364.35

Physical Properties

Property code	Value	Unit	Source
gf	-962.81	kJ/mol	Joback Method
hf	-1343.80	kJ/mol	Joback Method
hfus	52.86	kJ/mol	Joback Method
hvap	66.28	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	5.846		Crippen Method
mcvol	252.710	ml/mol	McGowan Method
pc	1260.16	kPa	Joback Method
rinpol	1909.00		NIST Webbook
tb	739.62	K	Joback Method
tc	915.68	K	Joback Method
tf	451.67	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.07	J/mol×K	739.62	Joback Method
cpg	738.32	J/mol×K	768.96	Joback Method
cpg	751.83	J/mol×K	798.31	Joback Method
cpg	764.64	J/mol×K	827.65	Joback Method
cpg	776.76	J/mol×K	857.00	Joback Method
cpg	788.21	J/mol×K	886.34	Joback Method
cpg	799.00	J/mol×K	915.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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