Pentafluorobenzoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C18H17F5O2/c1-5-6-10(4)11(8-7-9(2)3)25-18(24)12-13(19)15(21)17(23)16(22

InchiKey: JMJZILCDXAMXNO-UHFFFAOYSA-N

Formula: C18H17F5O2

SMILES: C=C(C)C#CC(OC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)CCC

Mol. weight [g/mol]: 360.32

Physical Properties

Property code	Value	Unit	Source
gf	-765.82	kJ/mol	Joback Method
hf	-1083.64	kJ/mol	Joback Method
hfus	46.14	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	4.923		Crippen Method
mcvol	244.110	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
tb	740.14	K	Joback Method
tc	930.59	K	Joback Method
tf	517.13	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.95	J/mol×K	740.14	Joback Method
cpg	690.85	J/mol×K	771.88	Joback Method
cpg	703.96	J/mol×K	803.62	Joback Method
cpg	716.29	J/mol×K	835.37	Joback Method
cpg	727.86	J/mol×K	867.11	Joback Method
cpg	738.68	J/mol×K	898.85	Joback Method
cpg	748.76	J/mol×K	930.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299188&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume