Pentafluorobenzoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C17H15F5O2/c1-8(2)5-6-10(7-9(3)4)24-17(23)11-12(18)14(20)16(22)15(21)13

InchiKey: XSVXMGNYSMOXGA-UHFFFAOYSA-N

Formula: C17H15F5O2

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

Mol. weight [g/mol]: 346.29

Physical Properties

Property code	Value	Unit	Source
gf	-774.24	kJ/mol	Joback Method
hf	-1063.00	kJ/mol	Joback Method
hfus	43.55	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	4.533		Crippen Method
mcvol	230.020	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	1612.00		NIST Webbook
tb	717.26	K	Joback Method
tc	908.56	K	Joback Method
tf	505.86	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.79	J/mol×K	717.26	Joback Method
cpg	636.24	J/mol×K	749.14	Joback Method
cpg	648.93	J/mol×K	781.03	Joback Method
cpg	660.89	J/mol×K	812.91	Joback Method
cpg	672.11	J/mol×K	844.79	Joback Method
cpg	682.62	J/mol×K	876.67	Joback Method
cpg	692.42	J/mol×K	908.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299187&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

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