Pentafluorobenzoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C16H15F5O2/c1-4-5-6-9(7-8(2)3)23-16(22)10-11(17)13(19)15(21)14(20)12(10
InchiKey: NXRDZCWQHUQIGX-UHFFFAOYSA-N
Formula: C16H15F5O2
SMILES: CCC#CC(CC(C)C)OC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 334.28

Physical Properties

Property code	Value	Unit	Source
gf	-861.95	kJ/mol	Joback Method
hf	-1158.00	kJ/mol	Joback Method
hfus	43.55	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	4.367		Crippen Method
mcvol	220.230	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	1568.00		NIST Webbook
rinpol	1568.00		NIST Webbook
tb	697.82	K	Joback Method
tc	885.47	K	Joback Method
tf	510.31	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.74	J/mol×K	697.82	Joback Method
cpg	607.11	J/mol×K	729.10	Joback Method
cpg	619.78	J/mol×K	760.37	Joback Method
cpg	631.75	J/mol×K	791.65	Joback Method
cpg	643.02	J/mol×K	822.92	Joback Method
cpg	653.59	J/mol×K	854.20	Joback Method
cpg	663.48	J/mol×K	885.47	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=U299186&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume