Pentafluorobenzoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C20H23F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-27-20(26)14-15(21)17(23)19(25
InchiKey: OOSBOESRAMWXPK-UHFFFAOYSA-N
Formula: C20H23F5O2
SMILES: CCCCCCCCCCC#CCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 390.39

Physical Properties

Property code	Value	Unit	Source
gf	-823.39	kJ/mol	Joback Method
hf	-1230.00	kJ/mol	Joback Method
hfus	60.96	kJ/mol	Joback Method
hvap	72.92	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	6.073		Crippen Method
mcvol	276.590	ml/mol	McGowan Method
pc	1188.24	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	790.22	K	Joback Method
tc	974.96	K	Joback Method
tf	585.39	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.97	J/mol×K	790.22	Joback Method
cpg	828.87	J/mol×K	821.01	Joback Method
cpg	842.93	J/mol×K	851.80	Joback Method
cpg	856.16	J/mol×K	882.59	Joback Method
cpg	868.56	J/mol×K	913.38	Joback Method
cpg	880.16	J/mol×K	944.17	Joback Method
cpg	890.96	J/mol×K	974.96	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=U299190&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