3-Trifluoromethylbenzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C14H4F8O2/c15-7-8(16)10(18)12(11(19)9(7)17)24-13(23)5-2-1-3-6(4-5)14(20,
InchiKey: ILMCTCNCFZTPCZ-UHFFFAOYSA-N
Formula: C14H4F8O2
SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 356.17

Physical Properties

Property code	Value	Unit	Source
gf	-1555.52	kJ/mol	Joback Method
hf	-1750.48	kJ/mol	Joback Method
hfus	37.78	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	4.620		Crippen Method
mcvol	182.200	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1461.00		NIST Webbook
rinpol	1461.00		NIST Webbook
tb	670.18	K	Joback Method
tc	856.37	K	Joback Method
tf	454.80	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.08	J/mol×K	670.18	Joback Method
cpg	487.00	J/mol×K	701.21	Joback Method
cpg	496.26	J/mol×K	732.24	Joback Method
cpg	504.89	J/mol×K	763.28	Joback Method
cpg	512.90	J/mol×K	794.31	Joback Method
cpg	520.31	J/mol×K	825.34	Joback Method
cpg	527.15	J/mol×K	856.37	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=U355139&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