2,4,6-Trimethylphenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C16H11F5O2/c1-6-4-7(2)15(8(3)5-6)23-16(22)9-10(17)12(19)14(21)13(20)11(9
InchiKey: GGJGIIHZEAAWPT-UHFFFAOYSA-N
Formula: C16H11F5O2
SMILES: Cc1cc(C)c(OC(=O)c2c(F)c(F)c(F)c(F)c2F)c(C)c1
Mol. weight [g/mol]: 330.25

Physical Properties

Property code	Value	Unit	Source
gf	-976.35	kJ/mol	Joback Method
hf	-1217.62	kJ/mol	Joback Method
hfus	40.35	kJ/mol	Joback Method
hvap	66.13	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	4.527		Crippen Method
mcvol	205.070	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	1728.00		NIST Webbook
rinpol	1731.30		NIST Webbook
rinpol	1735.60		NIST Webbook
rinpol	1728.00		NIST Webbook
tb	731.32	K	Joback Method
tc	928.38	K	Joback Method
tf	498.19	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.91	J/mol×K	731.32	Joback Method
cpg	561.85	J/mol×K	764.16	Joback Method
cpg	573.08	J/mol×K	797.01	Joback Method
cpg	583.57	J/mol×K	829.85	Joback Method
cpg	593.34	J/mol×K	862.69	Joback Method
cpg	602.38	J/mol×K	895.54	Joback Method

cpg	610.69	J/mol×K	928.38	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=R433020&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