4(1,1-Dimethylbutyl)phenol, pentafluorobenzoyl ester

Inchi: InChI=1S/C19H17F5O2/c1-4-9-19(2,3)10-5-7-11(8-6-10)26-18(25)12-13(20)15(22)17(24
InchiKey: OAZHPWDYKBFPII-UHFFFAOYSA-N
Formula: C19H17F5O2
SMILES: CCCC(C)(C)c1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]: 372.33

Physical Properties

Property code	Value	Unit	Source
gf	-928.99	kJ/mol	Joback Method
hf	-1265.35	kJ/mol	Joback Method
hfus	41.49	kJ/mol	Joback Method
hvap	70.19	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	5.679		Crippen Method
mcvol	247.340	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinpol	1984.40		NIST Webbook
rinpol	1992.60		NIST Webbook
rinpol	1987.80		NIST Webbook
rinpol	1984.40		NIST Webbook
tb	786.77	K	Joback Method
tc	986.29	K	Joback Method
tf	509.38	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.98	J/mol×K	786.77	Joback Method
cpg	730.52	J/mol×K	820.02	Joback Method
cpg	743.14	J/mol×K	853.28	Joback Method
cpg	754.86	J/mol×K	886.53	Joback Method
cpg	765.73	J/mol×K	919.78	Joback Method
cpg	775.76	J/mol×K	953.04	Joback Method

cpg	785.01	J/mol×K	986.29	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=R433248&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

Latest version available from:
https://www.chemeo.com/cid/121-743-2/4-1-1-Dimethylbutyl-phenol-pentafluorobenzoyl-ester.pdf
Generated by Cheméo on 2024-04-27 17:48:45.54313094 +0000 UTC m=+16529374.463708251.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.