Fumaric acid, di(pentafluorobenzyl) ester

Inchi: InChI=1S/C18H6F10O4/c19-9-5(10(20)14(24)17(27)13(9)23)3-31-7(29)1-2-8(30)32-4-6-1
InchiKey: IIQZBSJRHSWMSU-OWOJBTEDSA-N
Formula: C18H6F10O4
SMILES: O=C(C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 476.22

Physical Properties

Property code	Value	Unit	Source
gf	-2106.52	kJ/mol	Joback Method
hf	-2389.97	kJ/mol	Joback Method
hfus	63.14	kJ/mol	Joback Method
hvap	76.93	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	4.420		Crippen Method
mcvol	245.240	ml/mol	McGowan Method
pc	1331.98	kPa	Joback Method
rinpol	2146.00		NIST Webbook
rinpol	2146.00		NIST Webbook
tb	863.84	K	Joback Method
tc	1058.51	K	Joback Method
tf	615.80	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.94	J/mol×K	863.84	Joback Method
cpg	712.05	J/mol×K	896.28	Joback Method
cpg	720.34	J/mol×K	928.73	Joback Method
cpg	727.81	J/mol×K	961.17	Joback Method
cpg	734.46	J/mol×K	993.62	Joback Method
cpg	740.28	J/mol×K	1026.06	Joback Method
cpg	745.27	J/mol×K	1058.51	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=U405889&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