Fumaric acid, pentafluorobenzyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C17H17F5O4/c1-4-10(8(2)3)26-12(24)6-5-11(23)25-7-9-13(18)15(20)17(22)16

InchiKey: KIFJHVPUFQAYHM-AATRIKPKSA-N

Formula: C17H17F5O4

SMILES: CCC(OC(=O)C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F)C(C)C

Mol. weight [g/mol]: 380.31

Physical Properties

Property code	Value	Unit	Source
gf	-1210.03	kJ/mol	Joback Method
hf	-1578.52	kJ/mol	Joback Method
hfus	46.01	kJ/mol	Joback Method
hvap	72.43	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	3.959		Crippen Method
mcvol	246.060	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1925.00		NIST Webbook
tb	792.15	K	Joback Method
tc	980.17	K	Joback Method
tf	482.56	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.70	J/mol×K	792.15	Joback Method
cpg	727.34	J/mol×K	823.49	Joback Method
cpg	739.16	J/mol×K	854.82	Joback Method
cpg	750.18	J/mol×K	886.16	Joback Method
cpg	760.40	J/mol×K	917.50	Joback Method
cpg	769.82	J/mol×K	948.83	Joback Method
cpg	778.46	J/mol×K	980.17	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=U405877&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