Fumaric acid, pentafluorobenzyl dodec-2-en-1-yl ester

Inchi: InChI=1S/C23H27F5O4/c1-2-3-4-5-6-7-8-9-10-11-14-31-17(29)12-13-18(30)32-15-16-19

InchiKey: ZPQWPEBUOYMGNJ-AQASXUMVSA-N

Formula: C23H27F5O4

SMILES: CCCCCCCCCC=CCOC(=O)C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 462.45

Physical Properties

Property code	Value	Unit	Source
gf	-1074.41	kJ/mol	Joback Method
hf	-1574.58	kJ/mol	Joback Method
hfus	68.80	kJ/mol	Joback Method
hvap	86.52	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	6.222		Crippen Method
mcvol	326.300	ml/mol	McGowan Method
pc	977.17	kPa	Joback Method
rinpol	2639.00		NIST Webbook
rinpol	2639.00		NIST Webbook
tb	934.47	K	Joback Method
tc	1144.80	K	Joback Method
tf	575.10	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.75	J/mol×K	934.47	Joback Method
cpg	1049.50	J/mol×K	969.53	Joback Method
cpg	1063.14	J/mol×K	1004.58	Joback Method
cpg	1075.71	J/mol×K	1039.64	Joback Method
cpg	1087.25	J/mol×K	1074.69	Joback Method
cpg	1097.81	J/mol×K	1109.75	Joback Method
cpg	1107.41	J/mol×K	1144.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405887&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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