Fumaric acid, pentafluorobenzyl hept-2-yl ester

Inchi: InChI=1S/C18H19F5O4/c1-3-4-5-6-10(2)27-13(25)8-7-12(24)26-9-11-14(19)16(21)18(23

InchiKey: CXSPBNKQELSREN-BQYQJAHWSA-N

Formula: C18H19F5O4

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

Mol. weight [g/mol]: 394.33

Physical Properties

Property code	Value	Unit	Source
gf	-1199.17	kJ/mol	Joback Method
hf	-1593.88	kJ/mol	Joback Method
hfus	52.12	kJ/mol	Joback Method
hvap	75.05	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	4.494		Crippen Method
mcvol	260.150	ml/mol	McGowan Method
pc	1309.90	kPa	Joback Method
rinpol	2061.00		NIST Webbook
rinpol	2061.00		NIST Webbook
tb	815.47	K	Joback Method
tc	1003.83	K	Joback Method
tf	508.83	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.27	J/mol×K	815.47	Joback Method
cpg	783.26	J/mol×K	846.86	Joback Method
cpg	795.39	J/mol×K	878.26	Joback Method
cpg	806.68	J/mol×K	909.65	Joback Method
cpg	817.15	J/mol×K	941.04	Joback Method
cpg	826.79	J/mol×K	972.44	Joback Method
cpg	835.62	J/mol×K	1003.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405880&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

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