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

Inchi: InChI=1S/C17H19F5O4/c1-4-10(8(2)3)26-12(24)6-5-11(23)25-7-9-13(18)15(20)17(22)16

InchiKey: YFTRSBYKNYFSKZ-UHFFFAOYSA-N

Formula: C17H19F5O4

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

Mol. weight [g/mol]: 382.32

Physical Properties

Property code	Value	Unit	Source
gf	-1290.25	kJ/mol	Joback Method
hf	-1695.74	kJ/mol	Joback Method
hfus	45.81	kJ/mol	Joback Method
hvap	72.47	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.183		Crippen Method
mcvol	250.360	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	1891.00		NIST Webbook
rinpol	1891.00		NIST Webbook
tb	787.99	K	Joback Method
tc	972.51	K	Joback Method
tf	487.64	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.23	J/mol×K	787.99	Joback Method
cpg	753.44	J/mol×K	818.74	Joback Method
cpg	765.82	J/mol×K	849.50	Joback Method
cpg	777.34	J/mol×K	880.25	Joback Method
cpg	788.02	J/mol×K	911.01	Joback Method
cpg	797.84	J/mol×K	941.76	Joback Method
cpg	806.82	J/mol×K	972.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389880&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