Succinic acid, hept-2-yl pentafluorophenyl ester

Inchi: InChI=1S/C17H19F5O4/c1-3-4-5-6-9(2)25-10(23)7-8-11(24)26-17-15(21)13(19)12(18)14

InchiKey: DMARUPWVUFWYGW-UHFFFAOYSA-N

Formula: C17H19F5O4

SMILES: CCCCCC(C)OC(=O)CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 382.32

Physical Properties

Property code	Value	Unit	Source
gf	-1287.81	kJ/mol	Joback Method
hf	-1690.46	kJ/mol	Joback Method
hfus	49.33	kJ/mol	Joback Method
hvap	72.86	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	4.580		Crippen Method
mcvol	250.360	ml/mol	McGowan Method
pc	1352.64	kPa	Joback Method
rinpol	1832.00		NIST Webbook
rinpol	1832.00		NIST Webbook
tb	788.43	K	Joback Method
tc	971.70	K	Joback Method
tf	502.64	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.67	J/mol×K	788.43	Joback Method
cpg	752.80	J/mol×K	818.98	Joback Method
cpg	765.09	J/mol×K	849.52	Joback Method
cpg	776.56	J/mol×K	880.07	Joback Method
cpg	787.21	J/mol×K	910.61	Joback Method
cpg	797.02	J/mol×K	941.16	Joback Method
cpg	806.00	J/mol×K	971.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390350&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