Succinic acid, 5-fluoro-2-nitrophenyl pentafluorobenzyl ester

Inchi: InChI=1S/C17H9F6NO6/c18-7-1-2-9(24(27)28)10(5-7)30-12(26)4-3-11(25)29-6-8-13(19)

InchiKey: VZSGBCZDEHFGTP-UHFFFAOYSA-N

Formula: C17H9F6NO6

SMILES: O=C(CCC(=O)Oc1cc(F)ccc1[N+](=O)[O-])OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 437.25

Physical Properties

Property code	Value	Unit	Source
gf	-1351.48	kJ/mol	Joback Method
hf	-1678.46	kJ/mol	Joback Method
hfus	60.56	kJ/mol	Joback Method
hvap	92.62	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	3.858		Crippen Method
mcvol	245.790	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2464.00		NIST Webbook
rinpol	2464.00		NIST Webbook
tb	976.62	K	Joback Method
tc	1199.72	K	Joback Method
tf	713.30	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.06	J/mol×K	976.62	Joback Method
cpg	744.27	J/mol×K	1013.80	Joback Method
cpg	750.29	J/mol×K	1050.99	Joback Method
cpg	755.11	J/mol×K	1088.17	Joback Method
cpg	758.74	J/mol×K	1125.35	Joback Method
cpg	761.17	J/mol×K	1162.54	Joback Method
cpg	762.39	J/mol×K	1199.72	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=U357982&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