Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3-fluorophenyl ester

Inchi: InChI=1S/C15H11F9O4/c16-8-2-1-3-9(6-8)28-11(26)5-4-10(25)27-7-13(19,20)15(23,24)1

InchiKey: PBBFBHWPGXVPEA-UHFFFAOYSA-N

Formula: C15H11F9O4

SMILES: O=C(CCC(=O)Oc1cccc(F)c1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 426.23

Physical Properties

Property code	Value	Unit	Source
gf	-2036.85	kJ/mol	Joback Method
hf	-2413.99	kJ/mol	Joback Method
hfus	35.79	kJ/mol	Joback Method
hvap	58.61	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.225		Crippen Method
mcvol	229.260	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook
tb	710.14	K	Joback Method
tc	884.59	K	Joback Method
tf	439.64	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.47	J/mol×K	710.14	Joback Method
cpg	683.91	J/mol×K	739.22	Joback Method
cpg	694.54	J/mol×K	768.29	Joback Method
cpg	704.39	J/mol×K	797.37	Joback Method
cpg	713.50	J/mol×K	826.44	Joback Method
cpg	721.94	J/mol×K	855.52	Joback Method
cpg	729.73	J/mol×K	884.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390324&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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