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

Inchi: InChI=1S/C16H14F8O4/c1-9-4-2-3-5-10(9)28-12(26)7-6-11(25)27-8-14(19,20)16(23,24)1

InchiKey: LXPJDCNVHPKEON-UHFFFAOYSA-N

Formula: C16H14F8O4

SMILES: Cc1ccccc1OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 422.27

Physical Properties

Property code	Value	Unit	Source
gf	-1833.62	kJ/mol	Joback Method
hf	-2238.52	kJ/mol	Joback Method
hfus	35.30	kJ/mol	Joback Method
hvap	61.65	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.395		Crippen Method
mcvol	241.580	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	1838.00		NIST Webbook
rinpol	1838.00		NIST Webbook
tb	733.75	K	Joback Method
tc	913.20	K	Joback Method
tf	450.32	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.92	J/mol×K	733.75	Joback Method
cpg	730.10	J/mol×K	763.66	Joback Method
cpg	741.40	J/mol×K	793.57	Joback Method
cpg	751.88	J/mol×K	823.48	Joback Method
cpg	761.60	J/mol×K	853.39	Joback Method
cpg	770.60	J/mol×K	883.30	Joback Method
cpg	778.92	J/mol×K	913.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389758&Units=SI

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