Succinic acid, 3,5-dimethylphenyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C16H15F7O4/c1-9-5-10(2)7-11(6-9)27-13(25)4-3-12(24)26-8-14(17,18)15(19,2

InchiKey: GIEMKEUHISCYPL-UHFFFAOYSA-N

Formula: C16H15F7O4

SMILES: Cc1cc(C)cc(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F)c1

Mol. weight [g/mol]: 404.28

Physical Properties

Property code	Value	Unit	Source
gf	-1646.00	kJ/mol	Joback Method
hf	-2048.60	kJ/mol	Joback Method
hfus	35.35	kJ/mol	Joback Method
hvap	63.52	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.365		Crippen Method
mcvol	239.810	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	1769.00		NIST Webbook
rinpol	1769.00		NIST Webbook
tb	739.90	K	Joback Method
tc	922.86	K	Joback Method
tf	477.25	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.56	J/mol×K	739.90	Joback Method
cpg	720.85	J/mol×K	770.39	Joback Method
cpg	732.28	J/mol×K	800.89	Joback Method
cpg	742.89	J/mol×K	831.38	Joback Method
cpg	752.75	J/mol×K	861.87	Joback Method
cpg	761.88	J/mol×K	892.36	Joback Method
cpg	770.35	J/mol×K	922.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360725&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