Succinic acid, phenethyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C16H15F7O4/c17-14(18,15(19,20)16(21,22)23)10-27-13(25)7-6-12(24)26-9-8-

InchiKey: SLNYNXNPQFBTJC-UHFFFAOYSA-N

Formula: C16H15F7O4

SMILES: O=C(CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F)OCCc1ccccc1

Mol. weight [g/mol]: 404.28

Physical Properties

Property code	Value	Unit	Source
gf	-1626.74	kJ/mol	Joback Method
hf	-2025.66	kJ/mol	Joback Method
hfus	36.13	kJ/mol	Joback Method
hvap	62.19	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.929		Crippen Method
mcvol	239.810	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	1787.00		NIST Webbook
rinpol	1787.00		NIST Webbook
tb	729.94	K	Joback Method
tc	911.17	K	Joback Method
tf	452.21	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.52	J/mol×K	729.94	Joback Method
cpg	723.05	J/mol×K	760.14	Joback Method
cpg	734.68	J/mol×K	790.35	Joback Method
cpg	745.47	J/mol×K	820.55	Joback Method
cpg	755.47	J/mol×K	850.76	Joback Method
cpg	764.74	J/mol×K	880.96	Joback Method
cpg	773.33	J/mol×K	911.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357999&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