Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 1-cyclopentylethyl ester

Inchi: InChI=1S/C16H20F8O4/c1-9(10-4-2-3-5-10)28-12(26)7-6-11(25)27-8-14(19,20)16(23,24)15(21,22)13(17,18)

InchiKey: XKCIFUDFXRTBSO-UHFFFAOYSA-N

Formula: C16H20F8O4

SMILES: CC(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)C1CCCC1

Mol. weight [g/mol]: 428.31

Physical Properties

Property code	Value	Unit	Source
gf	-1902.29	kJ/mol	Joback Method
hf	-2408.38	kJ/mol	Joback Method
hfus	32.06	kJ/mol	Joback Method
hvap	58.58	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.603		Crippen Method
mcvol	254.480	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	1769.00		NIST Webbook
rinpol	1769.00		NIST Webbook
tb	716.93	K	Joback Method
tc	890.49	K	Joback Method
tf	407.28	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.59	J/mol×K	716.93	Joback Method
cpg	809.59	J/mol×K	745.86	Joback Method
cpg	823.63	J/mol×K	774.78	Joback Method
cpg	836.73	J/mol×K	803.71	Joback Method
cpg	848.96	J/mol×K	832.63	Joback Method
cpg	860.37	J/mol×K	861.56	Joback Method
cpg	871.01	J/mol×K	890.49	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=U391408&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