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

Inchi: InChI=1S/C17H22F8O4/c18-14(19)16(22,23)17(24,25)15(20,21)10-29-13(27)7-6-12(26)2

InchiKey: QJTKQNWQAAGEDL-UHFFFAOYSA-N

Formula: C17H22F8O4

SMILES: O=C(CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCCC1CCCCC1

Mol. weight [g/mol]: 442.34

Physical Properties

Property code	Value	Unit	Source
gf	-1903.53	kJ/mol	Joback Method
hf	-2429.90	kJ/mol	Joback Method
hfus	36.07	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.994		Crippen Method
mcvol	268.570	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	1928.00		NIST Webbook
rinpol	1928.00		NIST Webbook
tb	744.52	K	Joback Method
tc	920.82	K	Joback Method
tf	430.03	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.87	J/mol×K	744.52	Joback Method
cpg	869.39	J/mol×K	773.90	Joback Method
cpg	883.88	J/mol×K	803.29	Joback Method
cpg	897.38	J/mol×K	832.67	Joback Method
cpg	909.95	J/mol×K	862.05	Joback Method
cpg	921.63	J/mol×K	891.43	Joback Method
cpg	932.49	J/mol×K	920.82	Joback Method

Sources

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=U391392&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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