Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl trans-4-methylcyclohexyl ester

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

InchiKey: TYJAEFVTVKIEHJ-UHFFFAOYSA-N

Formula: C16H20F8O4

SMILES: CC1CCC(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)CC1

Mol. weight [g/mol]: 428.31

Physical Properties

Property code	Value	Unit	Source
gf	-1919.66	kJ/mol	Joback Method
hf	-2429.60	kJ/mol	Joback Method
hfus	34.55	kJ/mol	Joback Method
hvap	58.83	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.603		Crippen Method
mcvol	254.480	ml/mol	McGowan Method
pc	1289.29	kPa	Joback Method
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook
tb	716.97	K	Joback Method
tc	891.56	K	Joback Method
tf	414.52	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.74	J/mol×K	716.97	Joback Method
cpg	815.39	J/mol×K	746.07	Joback Method
cpg	830.01	J/mol×K	775.17	Joback Method
cpg	843.65	J/mol×K	804.27	Joback Method
cpg	856.34	J/mol×K	833.36	Joback Method
cpg	868.14	J/mol×K	862.46	Joback Method
cpg	879.08	J/mol×K	891.56	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=U390067&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