Succinic acid, 8-chlorooctyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C16H23ClF6O4/c17-9-5-3-1-2-4-6-10-26-12(24)7-8-13(25)27-11-15(19,20)14(1

InchiKey: GFKGRKKVQLHTSE-UHFFFAOYSA-N

Formula: C16H23ClF6O4

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

Mol. weight [g/mol]: 428.80

Physical Properties

Property code	Value	Unit	Source
gf	-1561.55	kJ/mol	Joback Method
hf	-2078.35	kJ/mol	Joback Method
hfus	47.10	kJ/mol	Joback Method
hvap	66.03	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.968		Crippen Method
mcvol	274.040	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	2062.00		NIST Webbook
rinpol	2062.00		NIST Webbook
tb	744.21	K	Joback Method
tc	914.90	K	Joback Method
tf	437.70	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.31	J/mol×K	744.21	Joback Method
cpg	829.23	J/mol×K	772.66	Joback Method
cpg	842.33	J/mol×K	801.11	Joback Method
cpg	854.66	J/mol×K	829.56	Joback Method
cpg	866.24	J/mol×K	858.01	Joback Method
cpg	877.10	J/mol×K	886.45	Joback Method
cpg	887.28	J/mol×K	914.90	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=U390812&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