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

Inchi: InChI=1S/C16H23F7O4/c1-2-3-4-5-6-7-10-26-12(24)8-9-13(25)27-11-14(17,18)15(19,20)

InchiKey: YVFXZPNCHRNERW-UHFFFAOYSA-N

Formula: C16H23F7O4

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

Mol. weight [g/mol]: 412.34

Physical Properties

Property code	Value	Unit	Source
gf	-1739.15	kJ/mol	Joback Method
hf	-2262.19	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	59.92	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.046		Crippen Method
mcvol	263.570	ml/mol	McGowan Method
pc	1172.83	kPa	Joback Method
rinpol	1677.00		NIST Webbook
rinpol	1677.00		NIST Webbook
tb	703.26	K	Joback Method
tc	866.49	K	Joback Method
tf	425.79	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.63	J/mol×K	703.26	Joback Method
cpg	809.01	J/mol×K	730.46	Joback Method
cpg	822.57	J/mol×K	757.67	Joback Method
cpg	835.37	J/mol×K	784.87	Joback Method
cpg	847.43	J/mol×K	812.08	Joback Method
cpg	858.80	J/mol×K	839.28	Joback Method
cpg	869.51	J/mol×K	866.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382355&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