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

Inchi: InChI=1S/C18H27F7O4/c1-2-3-4-5-6-7-8-9-12-28-14(26)10-11-15(27)29-13-16(19,20)17

InchiKey: DRBXDEQLCOAYDU-UHFFFAOYSA-N

Formula: C18H27F7O4

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

Mol. weight [g/mol]: 440.39

Physical Properties

Property code	Value	Unit	Source
gf	-1722.31	kJ/mol	Joback Method
hf	-2303.47	kJ/mol	Joback Method
hfus	47.27	kJ/mol	Joback Method
hvap	64.37	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.827		Crippen Method
mcvol	291.750	ml/mol	McGowan Method
pc	1032.57	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	749.02	K	Joback Method
tc	918.33	K	Joback Method
tf	448.33	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.80	J/mol×K	749.02	Joback Method
cpg	923.16	J/mol×K	777.24	Joback Method
cpg	937.63	J/mol×K	805.46	Joback Method
cpg	951.27	J/mol×K	833.67	Joback Method
cpg	964.10	J/mol×K	861.89	Joback Method
cpg	976.18	J/mol×K	890.11	Joback Method
cpg	987.56	J/mol×K	918.33	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=U382357&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