Succinic acid, hept-2-yl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C15H22F6O4/c1-3-4-5-6-10(2)25-12(23)8-7-11(22)24-9-14(17,18)13(16)15(19

InchiKey: ZATAQUQZXJEFTG-UHFFFAOYSA-N

Formula: C15H22F6O4

SMILES: CCCCCC(C)OC(=O)CCC(=O)OCC(F)(F)C(F)C(F)(F)F

Mol. weight [g/mol]: 380.32

Physical Properties

Property code	Value	Unit	Source
gf	-1560.48	kJ/mol	Joback Method
hf	-2047.25	kJ/mol	Joback Method
hfus	36.79	kJ/mol	Joback Method
hvap	59.03	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.357		Crippen Method
mcvol	247.710	ml/mol	McGowan Method
pc	1292.07	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	683.46	K	Joback Method
tc	847.03	K	Joback Method
tf	381.51	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.14	J/mol×K	683.46	Joback Method
cpg	744.53	J/mol×K	710.72	Joback Method
cpg	758.14	J/mol×K	737.98	Joback Method
cpg	771.00	J/mol×K	765.25	Joback Method
cpg	783.14	J/mol×K	792.51	Joback Method
cpg	794.59	J/mol×K	819.77	Joback Method
cpg	805.36	J/mol×K	847.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390803&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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