Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl cis-hex-2-en-1-yl ester

Inchi: InChI=1S/C15H18F8O4/c1-2-3-4-5-8-26-10(24)6-7-11(25)27-9-13(18,19)15(22,23)14(20

InchiKey: FBDTYFDVLNJAFU-PLNGDYQASA-N

Formula: C15H18F8O4

SMILES: CCCC=CCOC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 414.29

Physical Properties

Property code	Value	Unit	Source
gf	-1864.60	kJ/mol	Joback Method
hf	-2325.72	kJ/mol	Joback Method
hfus	39.26	kJ/mol	Joback Method
hvap	56.44	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.380		Crippen Method
mcvol	246.950	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
tb	683.37	K	Joback Method
tc	845.85	K	Joback Method
tf	395.03	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.64	J/mol×K	683.37	Joback Method
cpg	738.76	J/mol×K	710.45	Joback Method
cpg	751.11	J/mol×K	737.53	Joback Method
cpg	762.74	J/mol×K	764.61	Joback Method
cpg	773.67	J/mol×K	791.69	Joback Method
cpg	783.95	J/mol×K	818.77	Joback Method
cpg	793.62	J/mol×K	845.85	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=U391295&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