Succinic acid, 2-(adamant-1-yl)ethyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C21H26F8O4/c22-17(23)20(26,27)21(28,29)19(24,25)11-33-16(31)2-1-15(30)3

InchiKey: KFTXBKLYZRXBCK-UHFFFAOYSA-N

Formula: C21H26F8O4

SMILES: O=C(CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 494.42

Physical Properties

Property code	Value	Unit	Source
gf	-1737.35	kJ/mol	Joback Method
hf	-2359.64	kJ/mol	Joback Method
hfus	41.67	kJ/mol	Joback Method
hvap	68.29	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.630		Crippen Method
mcvol	303.210	ml/mol	McGowan Method
pc	1103.74	kPa	Joback Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
tb	836.55	K	Joback Method
tc	1027.61	K	Joback Method
tf	537.69	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1047.32	J/mol×K	836.55	Joback Method
cpg	1064.85	J/mol×K	868.39	Joback Method
cpg	1081.92	J/mol×K	900.24	Joback Method
cpg	1098.68	J/mol×K	932.08	Joback Method
cpg	1115.33	J/mol×K	963.93	Joback Method
cpg	1132.03	J/mol×K	995.77	Joback Method
cpg	1148.97	J/mol×K	1027.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391362&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