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

Inchi: InChI=1S/C20H24F8O4/c21-16(22)19(25,26)20(27,28)18(23,24)10-32-15(30)2-1-14(29)3

InchiKey: VHOHIGFNOVKEHP-UHFFFAOYSA-N

Formula: C20H24F8O4

SMILES: O=C(CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 480.39

Physical Properties

Property code	Value	Unit	Source
gf	-1745.77	kJ/mol	Joback Method
hf	-2339.00	kJ/mol	Joback Method
hfus	39.08	kJ/mol	Joback Method
hvap	66.06	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.240		Crippen Method
mcvol	289.120	ml/mol	McGowan Method
pc	1177.66	kPa	Joback Method
rinpol	2258.00		NIST Webbook
rinpol	2258.00		NIST Webbook
tb	813.67	K	Joback Method
tc	1002.38	K	Joback Method
tf	526.42	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.55	J/mol×K	813.67	Joback Method
cpg	1004.39	J/mol×K	845.12	Joback Method
cpg	1020.69	J/mol×K	876.57	Joback Method
cpg	1036.63	J/mol×K	908.03	Joback Method
cpg	1052.36	J/mol×K	939.48	Joback Method
cpg	1068.05	J/mol×K	970.93	Joback Method
cpg	1083.88	J/mol×K	1002.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391353&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