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

Inchi: InChI=1S/C22H28F8O4/c23-18(24)21(27,28)22(29,30)20(25,26)12-34-17(32)3-1-2-16(31

InchiKey: PSBIUOQDAZVVBN-UHFFFAOYSA-N

Formula: C22H28F8O4

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

Mol. weight [g/mol]: 508.44

Physical Properties

Property code	Value	Unit	Source
gf	-1728.93	kJ/mol	Joback Method
hf	-2380.28	kJ/mol	Joback Method
hfus	44.26	kJ/mol	Joback Method
hvap	70.52	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	6.021		Crippen Method
mcvol	317.300	ml/mol	McGowan Method
pc	1036.57	kPa	Joback Method
rinpol	2447.00		NIST Webbook
tb	859.43	K	Joback Method
tc	1053.62	K	Joback Method
tf	548.96	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.08	J/mol×K	859.43	Joback Method
cpg	1126.42	J/mol×K	891.80	Joback Method
cpg	1144.35	J/mol×K	924.16	Joback Method
cpg	1162.07	J/mol×K	956.53	Joback Method
cpg	1179.76	J/mol×K	988.89	Joback Method
cpg	1197.61	J/mol×K	1021.26	Joback Method
cpg	1215.81	J/mol×K	1053.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405375&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

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