Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C17H24F8O4/c1-9(2)13(10(3)4)29-12(27)7-5-6-11(26)28-8-15(20,21)17(24,25)

InchiKey: UZIDACGAFYRLDO-UHFFFAOYSA-N

Formula: C17H24F8O4

SMILES: CC(C)C(OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)C(C)C

Mol. weight [g/mol]: 444.36

Physical Properties

Property code	Value	Unit	Source
gf	-1935.30	kJ/mol	Joback Method
hf	-2500.06	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	59.77	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.095		Crippen Method
mcvol	279.430	ml/mol	McGowan Method
pc	1089.94	kPa	Joback Method
rinpol	1675.00		NIST Webbook
rinpol	1675.00		NIST Webbook
tb	723.65	K	Joback Method
tc	890.76	K	Joback Method
tf	377.65	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.44	J/mol×K	723.65	Joback Method
cpg	875.43	J/mol×K	751.50	Joback Method
cpg	889.52	J/mol×K	779.35	Joback Method
cpg	902.77	J/mol×K	807.20	Joback Method
cpg	915.20	J/mol×K	835.06	Joback Method
cpg	926.87	J/mol×K	862.91	Joback Method
cpg	937.82	J/mol×K	890.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393471&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