Glutaric acid, 1-cyclopentylethyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C17H22F8O4/c1-10(11-5-2-3-6-11)29-13(27)8-4-7-12(26)28-9-15(20,21)17(24

InchiKey: CSMXMGUVRRLWLA-UHFFFAOYSA-N

Formula: C17H22F8O4

SMILES: CC(OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)C1CCCC1

Mol. weight [g/mol]: 442.34

Physical Properties

Property code	Value	Unit	Source
gf	-1893.87	kJ/mol	Joback Method
hf	-2429.02	kJ/mol	Joback Method
hfus	34.65	kJ/mol	Joback Method
hvap	60.80	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.993		Crippen Method
mcvol	268.570	ml/mol	McGowan Method
pc	1218.29	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	739.81	K	Joback Method
tc	914.66	K	Joback Method
tf	418.55	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.96	J/mol×K	739.81	Joback Method
cpg	866.26	J/mol×K	768.95	Joback Method
cpg	880.57	J/mol×K	798.09	Joback Method
cpg	893.93	J/mol×K	827.24	Joback Method
cpg	906.41	J/mol×K	856.38	Joback Method
cpg	918.05	J/mol×K	885.52	Joback Method
cpg	928.92	J/mol×K	914.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405456&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