Glutaric acid, (cyclohex-3-enyl)methyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C17H20F8O4/c18-14(19)16(22,23)17(24,25)15(20,21)10-29-13(27)8-4-7-12(26

InchiKey: ZZTNROWWVMEVTL-UHFFFAOYSA-N

Formula: C17H20F8O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCC1CC=CCC1

Mol. weight [g/mol]: 440.33

Physical Properties

Property code	Value	Unit	Source
gf	-1873.57	kJ/mol	Joback Method
hf	-2372.12	kJ/mol	Joback Method
hfus	37.29	kJ/mol	Joback Method
hvap	61.66	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.770		Crippen Method
mcvol	264.270	ml/mol	McGowan Method
pc	1264.65	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	743.68	K	Joback Method
tc	920.54	K	Joback Method
tf	430.79	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.30	J/mol×K	743.68	Joback Method
cpg	843.04	J/mol×K	773.16	Joback Method
cpg	856.76	J/mol×K	802.63	Joback Method
cpg	869.54	J/mol×K	832.11	Joback Method
cpg	881.41	J/mol×K	861.58	Joback Method
cpg	892.44	J/mol×K	891.06	Joback Method
cpg	902.67	J/mol×K	920.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405522&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