Glutaric acid, di(2,2,3,4,4,4-hexafluorobutyl) ester

Inchi: InChI=1S/C13H12F12O4/c14-8(12(20,21)22)10(16,17)4-28-6(26)2-1-3-7(27)29-5-11(18,1

InchiKey: BSLAHWPDAIQDEQ-UHFFFAOYSA-N

Formula: C13H12F12O4

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

Mol. weight [g/mol]: 460.21

Physical Properties

Property code	Value	Unit	Source
gf	-2740.50	kJ/mol	Joback Method
hf	-3200.13	kJ/mol	Joback Method
hfus	35.26	kJ/mol	Joback Method
hvap	47.08	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.315		Crippen Method
mcvol	230.150	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook
tb	626.86	K	Joback Method
tc	774.40	K	Joback Method
tf	367.35	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.99	J/mol×K	626.86	Joback Method
cpg	688.93	J/mol×K	651.45	Joback Method
cpg	700.16	J/mol×K	676.04	Joback Method
cpg	710.71	J/mol×K	700.63	Joback Method
cpg	720.61	J/mol×K	725.22	Joback Method
cpg	729.89	J/mol×K	749.81	Joback Method
cpg	738.59	J/mol×K	774.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393700&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