Glutaric acid, 3-methylbut-2-en-1-yl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C14H18F6O4/c1-9(2)6-7-23-10(21)4-3-5-11(22)24-8-13(16,17)12(15)14(18,19)

InchiKey: HWADNWRUFGLELM-UHFFFAOYSA-N

Formula: C14H18F6O4

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

Mol. weight [g/mol]: 364.28

Physical Properties

Property code	Value	Unit	Source
gf	-1494.79	kJ/mol	Joback Method
hf	-1913.90	kJ/mol	Joback Method
hfus	36.61	kJ/mol	Joback Method
hvap	57.23	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.745		Crippen Method
mcvol	229.320	ml/mol	McGowan Method
pc	1438.07	kPa	Joback Method
rinpol	1558.00		NIST Webbook
rinpol	1558.00		NIST Webbook
tb	665.06	K	Joback Method
tc	831.21	K	Joback Method
tf	366.20	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.34	J/mol×K	665.06	Joback Method
cpg	666.63	J/mol×K	692.75	Joback Method
cpg	679.17	J/mol×K	720.44	Joback Method
cpg	691.01	J/mol×K	748.13	Joback Method
cpg	702.17	J/mol×K	775.82	Joback Method
cpg	712.69	J/mol×K	803.52	Joback Method
cpg	722.59	J/mol×K	831.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393685&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