Glutaric acid, 2-methylpent-3-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C14H21F5O4/c1-4-10(9(2)3)23-12(21)7-5-6-11(20)22-8-13(15,16)14(17,18)19/

InchiKey: MTZXVCSSSMGAGE-UHFFFAOYSA-N

Formula: C14H21F5O4

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

Mol. weight [g/mol]: 348.31

Physical Properties

Property code	Value	Unit	Source
gf	-1374.09	kJ/mol	Joback Method
hf	-1830.50	kJ/mol	Joback Method
hfus	31.12	kJ/mol	Joback Method
hvap	57.62	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.875		Crippen Method
mcvol	231.850	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	1405.00		NIST Webbook
rinpol	1405.00		NIST Webbook
tb	661.31	K	Joback Method
tc	827.94	K	Joback Method
tf	369.65	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.97	J/mol×K	661.31	Joback Method
cpg	682.30	J/mol×K	689.08	Joback Method
cpg	695.86	J/mol×K	716.85	Joback Method
cpg	708.67	J/mol×K	744.62	Joback Method
cpg	720.77	J/mol×K	772.40	Joback Method
cpg	732.17	J/mol×K	800.17	Joback Method
cpg	742.89	J/mol×K	827.94	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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