Glutaric acid, 2-methylpent-3-yl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C15H22F6O4/c1-4-10(9(2)3)25-12(23)7-5-6-11(22)24-8-14(17,18)13(16)15(19

InchiKey: YEGDETUHOKMQFB-UHFFFAOYSA-N

Formula: C15H22F6O4

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

Mol. weight [g/mol]: 380.32

Physical Properties

Property code	Value	Unit	Source
gf	-1562.92	kJ/mol	Joback Method
hf	-2052.53	kJ/mol	Joback Method
hfus	33.26	kJ/mol	Joback Method
hvap	58.64	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.213		Crippen Method
mcvol	247.710	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
tb	683.02	K	Joback Method
tc	848.07	K	Joback Method
tf	366.51	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.61	J/mol×K	683.02	Joback Method
cpg	745.16	J/mol×K	710.53	Joback Method
cpg	758.90	J/mol×K	738.04	Joback Method
cpg	771.89	J/mol×K	765.55	Joback Method
cpg	784.13	J/mol×K	793.06	Joback Method
cpg	795.65	J/mol×K	820.56	Joback Method
cpg	806.49	J/mol×K	848.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393684&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