Glutaric acid, 2,2,3,3,4,4,4-heptafluorobutyl isobutyl ester

Inchi: InChI=1S/C13H17F7O4/c1-8(2)6-23-9(21)4-3-5-10(22)24-7-11(14,15)12(16,17)13(18,19)

InchiKey: JFMGKEYQCBYYDN-UHFFFAOYSA-N

Formula: C13H17F7O4

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

Mol. weight [g/mol]: 370.26

Physical Properties

Property code	Value	Unit	Source
gf	-1766.85	kJ/mol	Joback Method
hf	-2205.55	kJ/mol	Joback Method
hfus	30.80	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.732		Crippen Method
mcvol	221.300	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpol	1497.00		NIST Webbook
rinpol	1497.00		NIST Webbook
tb	634.18	K	Joback Method
tc	794.40	K	Joback Method
tf	376.98	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.41	J/mol×K	634.18	Joback Method
cpg	646.58	J/mol×K	660.88	Joback Method
cpg	658.99	J/mol×K	687.59	Joback Method
cpg	670.70	J/mol×K	714.29	Joback Method
cpg	681.72	J/mol×K	741.00	Joback Method
cpg	692.09	J/mol×K	767.70	Joback Method
cpg	701.85	J/mol×K	794.40	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=U377547&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