Glutaric acid, 3-methylbut-2-en-1-yl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C13H18F4O4/c1-9(2)6-7-20-10(18)4-3-5-11(19)21-8-13(16,17)12(14)15/h6,12H

InchiKey: LDHLZJFWLWGNGI-UHFFFAOYSA-N

Formula: C13H18F4O4

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

Mol. weight [g/mol]: 314.27

Physical Properties

Property code	Value	Unit	Source
gf	-1116.43	kJ/mol	Joback Method
hf	-1492.29	kJ/mol	Joback Method
hfus	35.27	kJ/mol	Joback Method
hvap	57.93	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.110		Crippen Method
mcvol	211.690	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook
tb	646.87	K	Joback Method
tc	816.95	K	Joback Method
tf	351.33	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.97	J/mol×K	646.87	Joback Method
cpg	595.32	J/mol×K	675.22	Joback Method
cpg	607.98	J/mol×K	703.56	Joback Method
cpg	619.97	J/mol×K	731.91	Joback Method
cpg	631.32	J/mol×K	760.26	Joback Method
cpg	642.04	J/mol×K	788.60	Joback Method
cpg	652.17	J/mol×K	816.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393660&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