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

Inchi: InChI=1S/C13H19F3O4/c1-9(2)7-8-19-11(17)5-4-6-12(18)20-10(3)13(14,15)16/h7,10H,4

InchiKey: GFHZLCDKQUTHPB-UHFFFAOYSA-N

Formula: C13H19F3O4

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

Mol. weight [g/mol]: 296.28

Physical Properties

Property code	Value	Unit	Source
gf	-921.62	kJ/mol	Joback Method
hf	-1296.18	kJ/mol	Joback Method
hfus	32.19	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.160		Crippen Method
mcvol	209.920	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook
tb	647.60	K	Joback Method
tc	823.36	K	Joback Method
tf	350.74	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.96	J/mol×K	647.60	Joback Method
cpg	587.80	J/mol×K	676.89	Joback Method
cpg	600.91	J/mol×K	706.19	Joback Method
cpg	613.33	J/mol×K	735.48	Joback Method
cpg	625.06	J/mol×K	764.78	Joback Method
cpg	636.13	J/mol×K	794.07	Joback Method
cpg	646.58	J/mol×K	823.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393652&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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