Glutaric acid, hexa-1,5-dien-3-yl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C14H19F3O4/c1-4-7-11(5-2)21-13(19)9-6-8-12(18)20-10(3)14(15,16)17/h4-5,1

InchiKey: LIEUNBMBZIHMHY-UHFFFAOYSA-N

Formula: C14H19F3O4

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

Mol. weight [g/mol]: 308.29

Physical Properties

Property code	Value	Unit	Source
gf	-811.63	kJ/mol	Joback Method
hf	-1178.67	kJ/mol	Joback Method
hfus	29.81	kJ/mol	Joback Method
hvap	59.21	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.325		Crippen Method
mcvol	219.710	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1441.00		NIST Webbook
rinpol	1441.00		NIST Webbook
tb	659.36	K	Joback Method
tc	834.04	K	Joback Method
tf	362.53	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.53	J/mol×K	659.36	Joback Method
cpg	617.39	J/mol×K	688.47	Joback Method
cpg	630.50	J/mol×K	717.59	Joback Method
cpg	642.89	J/mol×K	746.70	Joback Method
cpg	654.57	J/mol×K	775.81	Joback Method
cpg	665.57	J/mol×K	804.93	Joback Method
cpg	675.92	J/mol×K	834.04	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=U405271&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