Glutaric acid, 3-methylbut-2-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C13H19F5O4/c1-8(2)9(3)22-11(20)6-4-5-10(19)21-7-12(14,15)13(16,17)18/h8-

InchiKey: QTRYUFBYUAGPRU-UHFFFAOYSA-N

Formula: C13H19F5O4

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

Mol. weight [g/mol]: 334.28

Physical Properties

Property code	Value	Unit	Source
gf	-1382.51	kJ/mol	Joback Method
hf	-1809.86	kJ/mol	Joback Method
hfus	28.53	kJ/mol	Joback Method
hvap	55.39	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.485		Crippen Method
mcvol	217.760	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
tb	638.43	K	Joback Method
tc	804.77	K	Joback Method
tf	358.38	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.90	J/mol×K	638.43	Joback Method
cpg	628.77	J/mol×K	666.15	Joback Method
cpg	641.90	J/mol×K	693.88	Joback Method
cpg	654.32	J/mol×K	721.60	Joback Method
cpg	666.03	J/mol×K	749.32	Joback Method
cpg	677.08	J/mol×K	777.05	Joback Method
cpg	687.48	J/mol×K	804.77	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=U393666&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