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

Inchi: InChI=1S/C13H20F4O4/c1-8(2)9(3)21-11(19)6-4-5-10(18)20-7-13(16,17)12(14)15/h8-9,1

InchiKey: OJUBNHICEBAOKN-UHFFFAOYSA-N

Formula: C13H20F4O4

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

Mol. weight [g/mol]: 316.29

Physical Properties

Property code	Value	Unit	Source
gf	-1192.98	kJ/mol	Joback Method
hf	-1610.28	kJ/mol	Joback Method
hfus	29.34	kJ/mol	Joback Method
hvap	57.12	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.188		Crippen Method
mcvol	215.990	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
tb	641.95	K	Joback Method
tc	809.65	K	Joback Method
tf	340.37	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.46	J/mol×K	641.95	Joback Method
cpg	618.64	J/mol×K	669.90	Joback Method
cpg	632.11	J/mol×K	697.85	Joback Method
cpg	644.88	J/mol×K	725.80	Joback Method
cpg	656.97	J/mol×K	753.75	Joback Method
cpg	668.40	J/mol×K	781.70	Joback Method
cpg	679.18	J/mol×K	809.65	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=U393564&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