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

Inchi: InChI=1S/C16H17F5O4/c1-7(2)8(3)24-9(22)5-4-6-10(23)25-16-14(20)12(18)11(17)13(19

InchiKey: MQMHMOPJILWVDF-UHFFFAOYSA-N

Formula: C16H17F5O4

SMILES: CC(C)C(C)OC(=O)CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 368.30

Physical Properties

Property code	Value	Unit	Source
gf	-1298.67	kJ/mol	Joback Method
hf	-1675.10	kJ/mol	Joback Method
hfus	43.22	kJ/mol	Joback Method
hvap	70.25	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.045		Crippen Method
mcvol	236.270	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	1739.00		NIST Webbook
rinpol	1739.00		NIST Webbook
tb	765.11	K	Joback Method
tc	948.27	K	Joback Method
tf	476.37	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.58	J/mol×K	765.11	Joback Method
cpg	697.36	J/mol×K	795.64	Joback Method
cpg	709.35	J/mol×K	826.16	Joback Method
cpg	720.55	J/mol×K	856.69	Joback Method
cpg	730.97	J/mol×K	887.22	Joback Method
cpg	740.59	J/mol×K	917.75	Joback Method
cpg	749.41	J/mol×K	948.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392106&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

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