Glutaric acid, 2-methylhex-3-yl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C20H25F5O4/c1-5-7-12(10(2)3)29-14(27)9-6-8-13(26)28-11(4)15-16(21)18(23

InchiKey: IKIZOJQVHHHMPO-UHFFFAOYSA-N

Formula: C20H25F5O4

SMILES: CCCC(OC(=O)CCCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F)C(C)C

Mol. weight [g/mol]: 424.40

Physical Properties

Property code	Value	Unit	Source
gf	-1267.43	kJ/mol	Joback Method
hf	-1762.94	kJ/mol	Joback Method
hfus	50.06	kJ/mol	Joback Method
hvap	78.76	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.524		Crippen Method
mcvol	292.630	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	856.19	K	Joback Method
tc	1049.49	K	Joback Method
tf	506.45	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.18	J/mol×K	856.19	Joback Method
cpg	927.65	J/mol×K	888.41	Joback Method
cpg	941.03	J/mol×K	920.62	Joback Method
cpg	953.34	J/mol×K	952.84	Joback Method
cpg	964.58	J/mol×K	985.06	Joback Method
cpg	974.75	J/mol×K	1017.27	Joback Method
cpg	983.85	J/mol×K	1049.49	Joback Method

Sources

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=U376999&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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