Glutaric acid, monocloride, pentafluorobenzyl ester

Inchi: InChI=1S/C12H8ClF5O3/c13-6(19)2-1-3-7(20)21-4-5-8(14)10(16)12(18)11(17)9(5)15/h1-

InchiKey: CERKZCLELURDSX-UHFFFAOYSA-N

Formula: C12H8ClF5O3

SMILES: O=C(Cl)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 330.63

Physical Properties

Property code	Value	Unit	Source
gf	-1234.40	kJ/mol	Joback Method
hf	-1465.50	kJ/mol	Joback Method
hfus	42.91	kJ/mol	Joback Method
hvap	64.09	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.361		Crippen Method
mcvol	186.280	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1728.00		NIST Webbook
tb	689.48	K	Joback Method
tc	872.25	K	Joback Method
tf	468.98	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.72	J/mol×K	689.48	Joback Method
cpg	481.34	J/mol×K	719.94	Joback Method
cpg	490.43	J/mol×K	750.40	Joback Method
cpg	498.99	J/mol×K	780.86	Joback Method
cpg	507.02	J/mol×K	811.32	Joback Method
cpg	514.51	J/mol×K	841.79	Joback Method
cpg	521.47	J/mol×K	872.25	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358885&Units=SI

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