Glutaric acid, 2-chloro-6-fluorophenyl pentafluorobenzyl ester

Inchi: InChI=1S/C18H11ClF6O4/c19-9-3-1-4-10(20)18(9)29-12(27)6-2-5-11(26)28-7-8-13(21)15

InchiKey: YLCQTLZZGVWWSL-UHFFFAOYSA-N

Formula: C18H11ClF6O4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 440.72

Physical Properties

Property code	Value	Unit	Source
gf	-1390.54	kJ/mol	Joback Method
hf	-1704.08	kJ/mol	Joback Method
hfus	55.99	kJ/mol	Joback Method
hvap	82.64	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	4.994		Crippen Method
mcvol	254.700	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2339.00		NIST Webbook
rinpol	2339.00		NIST Webbook
tb	885.09	K	Joback Method
tc	1089.57	K	Joback Method
tf	610.88	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.48	J/mol×K	885.09	Joback Method
cpg	736.21	J/mol×K	919.17	Joback Method
cpg	744.96	J/mol×K	953.25	Joback Method
cpg	752.73	J/mol×K	987.33	Joback Method
cpg	759.51	J/mol×K	1021.41	Joback Method
cpg	765.31	J/mol×K	1055.49	Joback Method
cpg	770.12	J/mol×K	1089.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391937&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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