Glutaric acid, 2,4,6-trichlorophenyl pentafluorobenzyl ester

Inchi: InChI=1S/C18H10Cl3F5O4/c19-7-4-9(20)18(10(21)5-7)30-12(28)3-1-2-11(27)29-6-8-13(

InchiKey: HAMSANOUJCSSOD-UHFFFAOYSA-N

Formula: C18H10Cl3F5O4

SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 491.62

Physical Properties

Property code	Value	Unit	Source
gf	-1229.22	kJ/mol	Joback Method
hf	-1550.92	kJ/mol	Joback Method
hfus	60.91	kJ/mol	Joback Method
hvap	92.89	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	6.161		Crippen Method
mcvol	277.410	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook
tb	965.66	K	Joback Method
tc	1186.00	K	Joback Method
tf	682.65	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.68	J/mol×K	965.66	Joback Method
cpg	762.25	J/mol×K	1002.38	Joback Method
cpg	768.69	J/mol×K	1039.11	Joback Method
cpg	774.00	J/mol×K	1075.83	Joback Method
cpg	778.16	J/mol×K	1112.55	Joback Method
cpg	781.18	J/mol×K	1149.28	Joback Method
cpg	783.05	J/mol×K	1186.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391942&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