Glutaric acid, 8-chlorooctyl pentafluorophenyl ester

Inchi: InChI=1S/C19H22ClF5O4/c20-10-5-3-1-2-4-6-11-28-12(26)8-7-9-13(27)29-19-17(24)15(2

InchiKey: DYBCFNUFZRJMLX-UHFFFAOYSA-N

Formula: C19H22ClF5O4

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

Mol. weight [g/mol]: 444.82

Physical Properties

Property code	Value	Unit	Source
gf	-1280.46	kJ/mol	Joback Method
hf	-1742.20	kJ/mol	Joback Method
hfus	62.23	kJ/mol	Joback Method
hvap	82.09	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.580		Crippen Method
mcvol	290.780	ml/mol	McGowan Method
pc	1144.44	kPa	Joback Method
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook
tb	872.06	K	Joback Method
tc	1067.87	K	Joback Method
tf	570.10	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.10	J/mol×K	872.06	Joback Method
cpg	892.17	J/mol×K	904.70	Joback Method
cpg	904.21	J/mol×K	937.33	Joback Method
cpg	915.24	J/mol×K	969.97	Joback Method
cpg	925.25	J/mol×K	1002.60	Joback Method
cpg	934.26	J/mol×K	1035.24	Joback Method
cpg	942.26	J/mol×K	1067.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392115&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