Glutaric acid, 8-chlorooctyl pentafluorobenzyl ester

Inchi: InChI=1S/C20H24ClF5O4/c21-10-5-3-1-2-4-6-11-29-14(27)8-7-9-15(28)30-12-13-16(22)
InchiKey: IMOXNQYILXPNMR-UHFFFAOYSA-N
Formula: C20H24ClF5O4
SMILES: O=C(CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F)OCCCCCCCCCCl
Mol. weight [g/mol]: 458.85

Physical Properties

Property code	Value	Unit	Source
gf	-1272.04	kJ/mol	Joback Method
hf	-1762.84	kJ/mol	Joback Method
hfus	64.82	kJ/mol	Joback Method
hvap	84.31	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	5.718		Crippen Method
mcvol	304.870	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	894.94	K	Joback Method
tc	1095.70	K	Joback Method
tf	581.37	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.44	J/mol×K	894.94	Joback Method
cpg	950.94	J/mol×K	928.40	Joback Method
cpg	963.32	J/mol×K	961.86	Joback Method
cpg	974.59	J/mol×K	995.32	Joback Method
cpg	984.76	J/mol×K	1028.78	Joback Method
cpg	993.84	J/mol×K	1062.24	Joback Method
cpg	1001.83	J/mol×K	1095.70	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=U391941&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